AEOLUS: Advances in Experimental Design, Optimal Control, and Learning for Uncertain Complex Systems
Center Progress Report: Year 3 (Oct 2020–Oct 2021)

Contents

1. Introduction

The AEOLUS Center is dedicated to developing a unified optimization-under-uncertainty framework for (1) **learning** predictive models from data and (2) **optimizing** experiments, processes, and designs governed by these models, all driven by complex, uncertain energy systems. AEOLUS will address the critical need for principled, rigorous, scalable, and structure-exploiting capabilities for exploring parameter and decision spaces of complex forward simulation models—the so-called **outer loop**.

This report summarizes key highlights in the third year of AEOLUS research. Of course, 15 pages is not sufficient to do justice to the many AEOLUS research advances over the past year. Aiming to strike a balance between breadth and depth, we have selected 16 highlights to feature here. The full spectrum of research is represented by the 56 publications that have appeared or have been accepted during the reporting period (Appendix C).

These highlights are organized under three sections. §2 features mathematical and computational research advances that have been tailored to the structure of our nanomaterials self-assembly driving problem, while §3 does the same for our additive manufacturing problem. Finally, §4 presents mathematical and computational research advances that are cross-cutting and applied more broadly.

2. New model formulations, optimal design and control, and model reduction, with application to nanomanufacturing

Here we describe research advances in SCFT and NLCH models (§2.1), optimal design (§2.2), reduced-order modeling (§2.3), and model inadequacy (§2.4) for directed self-assembly of block copolymer melts.

2.1. SCFT and phase field theory and algorithms

Researchers: Lianghao Cao (UT), Danial Faghihi (UB), Omar Ghattas (UT), J. Tinsley Oden (UT)

During the reporting period, we continued to investigate mathematical and computational models for the self-assembly of block copolymer melts. Our effort focused on the self-consistent field theory (SCFT) model. In our mathematical analysis of the SCFT model, we are able to re-derive, with mathematical rigor, the SCFT model from the particle-based statistical mechanics description of the diblock copolymer melts and identify the approximations made during the derivation [10]. We also developed strategies to improve the computational efficiency of numerical algorithms for solving the SCFT model [8]. First, we extended the semi-implicit Siedel scheme for solving the saddle point problem of the SCFT model, originally applicable only for spectral methods, to real space methods with arbitrary boundary conditions. Second, we reformulated the SCFT problem in the framework of PDE-constrained optimization and analyzed the well-posedness of the formulation. A second order (Newton) approach for accelerating existing gradient-based algorithms is proposed.

We extended the dynamical density functional theory, which shares similarities with the nonlocal Cahn-Hilliard model of phase change, for directed self-assembly of diblock copolymer. The extended model incorporates (1) thermal effects, (2) polymer-substrate interaction effects, and (3) a local mobility matrix. The resulting extended model produces realistic characterizations of the diblock copolymer morphology development driven by thermal annealing and local laser heating. A fast linear semi-implicit time-stepping scheme is developed. Together with the optimization under uncertainty methods developed within AEOLUS, this extended model opens the door to (1) managing the polymer synthesis time frame by optimal control of the annealing temperature, and (2) enabling real-time defect elimination by controlling the trajectory of laser heating based on X-ray scattering data.

2.2. Nonlocal Cahn-Hilliard-based optimal design

Researchers: Lianghao Cao (UT), Joshua Chen (UT), Peng Chen (UT), Omar Ghattas (UT), Dingcheng Luo (UT), J. Tinsley Oden (UT)

We investigated the optimal design problem in chemoepitaxy for the directed self-assembly (DSA)

(a) Target morphology **(b)** Optimal guidepost design **(c)** Equilibrium state

Figure 1: Three dimensional optimal design with 16 circular guideposts.

of block copolymer (BCP) melts. In the chemoepitaxy process, a chemically patterned substrate is used to guide the phase separation of BCP mixtures to form desirable morphologies. We adopted a forward phase field model based on the direct minimization of the Ohta-Kawasaki free energy functional with the addition of substrate interactions, as formulated in [9]. This leads to a PDE-constrained optimization problem in which we optimally design the substrate pattern to achieve a target morphology, while having sufficiently sparse features to attain manufacturing efficiency.

Our previous investigations revealed two key challenges. The first is the difficulty of achieving sparse and manufacturable substrate designs when considering the entire substrate field as the design variable. We observed that it is difficult to precisely enforce the sparsity conditions in the infinite-dimensional setting through penalty terms alone. The second challenge stems from the existence of multiple equilibrium states in the forward problem. The equilibrium state produced by the forward solver depends on the initial guess chosen for the free-energy minimization. Thus, a substrate design that is optimal for one initial guess may not be optimal for another. Moreover, for a fixed initial guess, the equilibrium states are also sensitive to the substrate design. Small changes in the substrate design may result in convergence to a very different equilibrium state.

In the past year, we addressed these two challenges. We considered a formulation of the optimal design problem in which the substrate design consists of a given number of guideposts—units of attractive substrate in a predefined shape. Optimization is then carried out over the locations of the guideposts with penalties on the distances between guideposts to achieve sparsity of the design features. In the existing literature, evolutionary algorithms are commonly used to optimize guidepost locations. However, these algorithms are extremely slow and heuristic in nature. We developed a fast second order (Newton) optimization method that employs the Hessian of the control objective (deviation from a target morphology) with respect to the locations of the guideposts to significantly reduce the number of iterations to convergence. The Hessian is computed through an efficient adjoint-based formulation.

We also proposed a computational strategy that addresses the difficulties presented by the multiple equilibrium states in a deterministic setting. During each optimization iteration, we warm-start the forward solver with the converged equilibrium state from the previous substrate design. This encourages the equilibrium states to remain within a particular basin of attraction, providing continuity and smoothness to the objective function. The reliability of the optimal design is then assessed at the end of the optimization procedure by solving the forward problem for samples of the initial guess field, drawn from an appropriate random field distribution.

Using various guideposts shapes, our computational strategy is able to produce optimal designs for a range of problems, with an example provided in Figure 1. The efficiencies of both the forward solver and the Hessian-based optimization method allow us to successfully solve the optimal design problems in 3D. These problems are intractable with optimization methods in practical use for this class of problems,

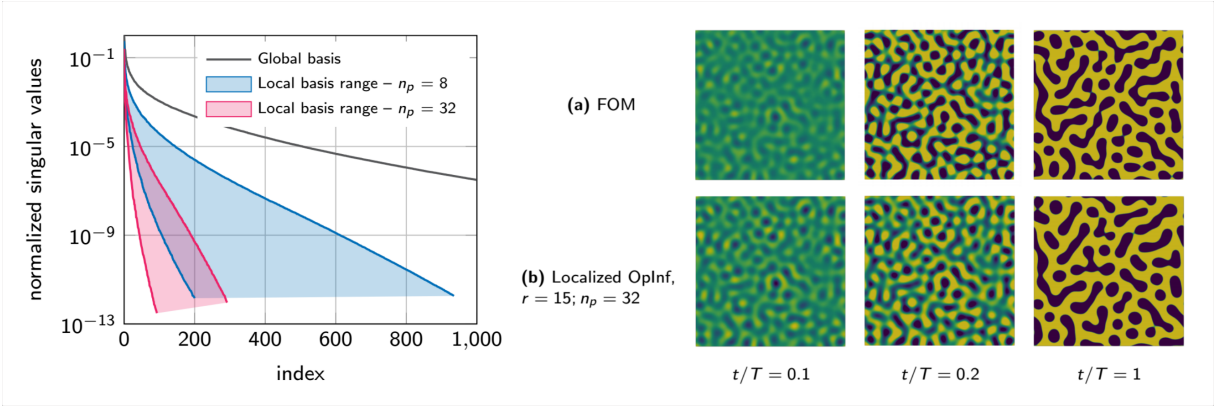


Figure 2: Localized reduced models using operator inference. Left: singular value decay of the training data is much faster when using localization. Right: Reduced model prediction (bottom) compared to the high-fidelity physics model (top).

which are derivative-free. Over the next year, we aim to systematically integrate uncertainties from both the initial state and physical parameters into the optimal design problem.

2.3. Model reduction for nonlocal Cahn-Hilliard

Researchers: Rudy Geelen (UT), Karen Willcox (UT)

Reduced-order modeling is a key enabling mathematical technology for tackling AEOLUS control and optimization target applications, but the Cahn-Hilliard phase-field model is widely recognized as a challenging problem for traditional model reduction techniques, due to the difficulty in finding a low-dimensional representation that captures the rich dynamics across multiple spatial and temporal scales. To address this challenge we have developed the localized operator inference approach, a new method for constructing *local* projection-based reduced models via data-driven learning directly from simulation data [22]. The novelty of the approach is to replace the global reduced basis with multiple local approximation subspaces. This localization permits adaptation of a reduced model to local dynamics, thereby keeping the reduced dimension small and leading to significant efficiency improvements. This is particularly important for reduced models of the Cahn-Hilliard equations, where the solution is typically characterized by different physical regimes and exhibits high sensitivity to parameter variations. Our new method differs from the existing literature in that the reduced models are learned in a completely non-intrusive fashion, meaning that they learn the reduced models from simulation data without requiring intrusive projections of high-fidelity model operators. This is an important consideration: the non-intrusive nature of localized operator inference makes the method accessible, portable, and applicable to a broad range of scientific problems, including those that use proprietary or legacy high-fidelity codes.

The localized operator inference approach follow a decomposition of computational tasks into two phases: the offline phase where the reduced model is derived from the high-fidelity physics model, and the online phase where the reduced model is deployed. The *offline* stage of the proposed approach consists of the following consecutive steps: (1) the training data are collected and partitioned into n_p groups/clusters of kinematically similar observations using unsupervised learning methods; (2) we train the classifier to recommend a good local reduced model with respect to a predefined indicator; (3) using operator inference we learn a set of cluster-specific reduced model operators. The reduced operators associated with each snapshot cluster define a cluster-specific reduced model. This leads to a set of n_p local reduced models that operate independently of one another. In the *online* phase of the approach (1) the indicator is computed and, using the classifier constructed in the offline stage, the most appropriate local reduced model is identified; (2) we evaluate the identified local reduced model to produce the approximate solution.

Figure 2 highlights the applicability of the proposed methodology in approximating, in a statistical sense, the leading order dynamics of phase separation as governed by the Cahn-Hilliard equation in an efficient manner. This is achieved by leveraging the low-rank local structure of the system: the singular values of the local POD bases decay faster than the singular values of the global basis. We also highlight the predictive capabilities of our reduced-order models when compared to high-dimensional physics-based models at selected time steps.

2.4. Model inadequacy

Researchers: Daniil Bochkov (UT), Robert Moser (UT), Todd Oliver (UT)

Significant progress has been made on the development of a low-intrusive methodology for inadequacy characterization for the class of physical models that can be represented mathematically as optimization problems, e.g., where a physically relevant solution is given by the system's energy minimum. The Self-Consistent Field Theory and the Ohta-Kawasaki phase-field model of block copolymer self-assembly are examples of this class. The proposed methodology is based on a posteriori error analysis. Specifically, the difference between low-fidelity and high-fidelity solutions is estimated using a quadratic approximation of the high-fidelity model around the low-fidelity solution in which, however, second-order derivatives are approximated by the low-fidelity model. The effect of such an approximation (compared to using exact second-order derivatives) is analyzed and expressed as a series involving powers of operator $D = H_0^{-1}H - I$, where H and H_0 are the Hessians of high-fidelity and low-fidelity models, respectively, acting on the solution difference $\Delta\boldsymbol{x}_0^*$ given by the quadratic approximation:

$$\Delta\boldsymbol{x}^* = \Delta\boldsymbol{x}_0^* - \frac{D\Delta\boldsymbol{x}_0^*}{1+\tilde{\lambda}} + \frac{D^2\Delta\boldsymbol{x}_0^* - \tilde{\lambda}D\Delta\boldsymbol{x}_0^*}{\left(1+\tilde{\lambda}\right)^2} - \frac{D^3\Delta\boldsymbol{x}_0^* - 2\tilde{\lambda}D^2\Delta\boldsymbol{x}_0^* + \tilde{\lambda}^2D\Delta\boldsymbol{x}_0^*}{\left(1+\tilde{\lambda}\right)^3} + \dots$$

where $\Delta\boldsymbol{x}^*$ is the solution difference when using exact second-order derivatives and $\tilde{\lambda}$ is an expansion parameter. We prove that due to the properties of D such a series can always be constructed to be convergent ($\tilde{\lambda} > \frac{\lambda_1 - 1}{2}$, where λ_1 is the largest positive eigenvalue of D) and use the first several terms to construct a stochastic inadequacy representation of a model.

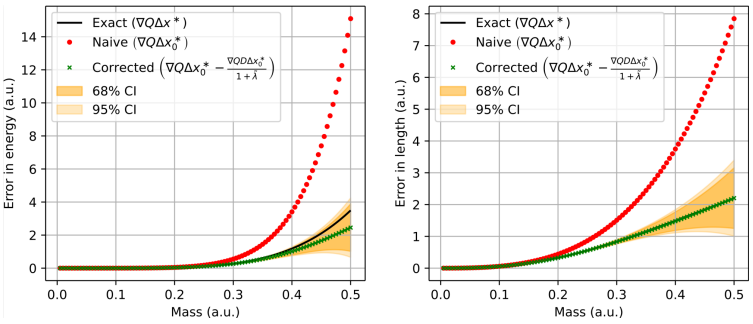


Figure 3: Characterization of errors in the system's energy and total chain length for test mass-spring model using proposed methodology.

The developed methodology has been tested on a simple physical system of a mass-spring chain with a nonlinear force-extension behavior, which is approximated by a linear dependence in the low-fidelity model. Representative results of applying the proposed methodology to this test system are shown in Figure 3 and demonstrate its ability to successfully characterize errors in QoIs.

Our future work in this direction will be focused on applying the developed approach to characterize model inadequacy in the context of simulating self-assembly of block copolymers.

3. Multiscale modeling and optimization, with application to additive manufacturing

In this section we describe research advances in multiscale modeling (§3.1) and nonlocal interface modeling (§3.2) for solidification in additive manufacturing.

3.1. Multiscale modeling in additive manufacturing

Researchers: Yuanxun Bao (UT), George Biros (UT), Stephen DeWitt (ORNL), Yigong Qin (UT) and Balasubramaniam Radhakrishnan (ORNL)

Additive manufacturing for metal alloys is revolutionizing the manufacturing industry by providing a process for creating near net shape parts with geometries that are hard to obtain with conventional processes. Additive manufacturing has the potential for specially tailored material properties in different areas of a part through control of the alloy composition and/or microstructure. However, to fully reap these benefits the processing conditions that lead to the desired local material properties must be found. A number of factors make the solidification conditions across an additively manufactured part heterogeneous, including variations in the local geometry, the feedstock, and the location relative to the scan path of the heat source. This heterogeneity makes the determination of process-structure-property connections challenging, even for a single part under nominally constant processing conditions. Determining the processing conditions that give locally tailored properties is even more challenging. An accurate and computationally efficient modeling framework to predict the effect of processing conditions on microstructure formation would be a significant step toward solving these challenges.

To address those challenges we have been pursuing several research directions for enabling control and uncertainty quantification in additive manufacturing systems. The first direction is the design of physics-based multiscale models for solidification. This effort is completed and we have submitted a paper to *Acta Materialia* [1]. The second direction is the formulation, analysis, and implementation of an optimization problem in which the heat source (laser) is designed to achieve an optimal microstructure. The third direction is the derivation of scientific machine learning algorithms for the development of reduced order models. These two last efforts are ongoing.

Our formulations are based on phase-field PDEs with varying degrees of fidelity. We have implemented parallel algorithms, with GPU acceleration, that enable direct numerical simulations of polycrystalline dendritic microstructure in full melt pools. We have also implemented simplified multicomponent phase-field models that capture individual grains. Although these models cannot capture the dendritic structure, they are over $10\times$ faster than the full resolution model and they capture coarse scale features of the solidification quite accurately. We have developed macroscale heat transfer simulations with semi-analytic models for the dendritic microstructure. Finally, we are developing deep neural networks that model the evolution of the microstructures. Below we summarize our work in physics-based multiscale modeling. Results on the optimization and ML-based reduced models will be reported next year.

We studied the epitaxial, columnar growth of (multiply oriented) dendrites/cells for a spot melt in a polycrystalline Al-Cu substrate using two-dimensional, phase-field, direct numerical simulations (DNS) at the full-melt-pool scale, as depicted in Figure 4. Our main objective is to compare the expensive DNS model to a much cheaper but approximate "line" model in which a single-crystal phase-field simulation is confined to a narrow rectangular geometry. To perform this comparison, we developed algorithms that automatically extract quantities of interest (QoIs) from both DNS and line models. These QoIs allow us to quantitatively assess the assumptions in the line model and help us analyze its discrepancy with the DNS model. We considered four sets of heat source parameters, mimicking welding and additive manufacturing conditions, that create a combination of shallow and deep melt pools. Our largest DNS simulation used 16K $\times$ 14K grid points in space. Our main findings can be summarized as follows. Under AM conditions, the QoIs of line models are in excellent agreement with the full DNS results for both shallow and deep melt pools. Under welding conditions, the primary spacing of the DNS model is

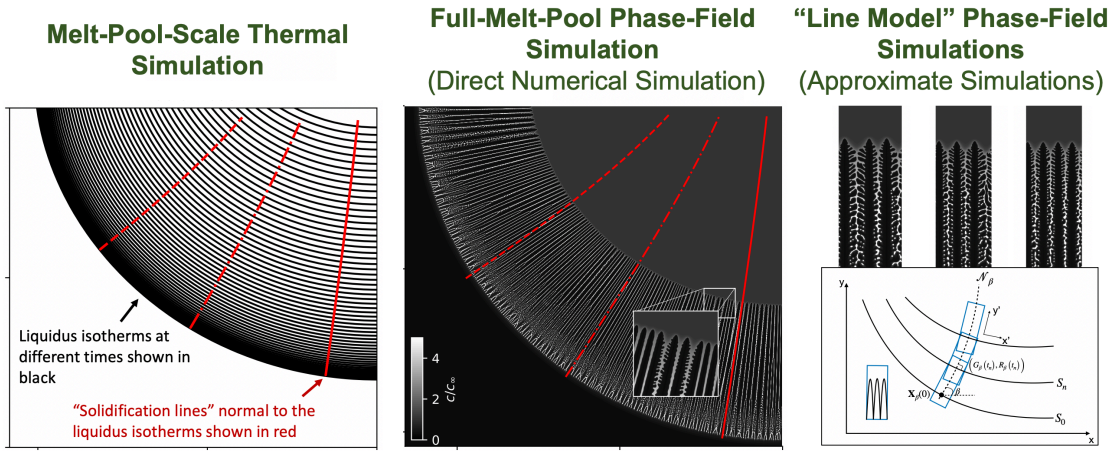


Figure 4: Multiscale models for AM. Left: melt-pool heat transfer to compute temperature evolution. Middle: DNS simulation of microstructure evolution. Right: Physics based reduced model.

smaller than the prediction of the line model. We identified a geometric crowding effect that accounts for the discrepancies between the DNS and line models. We proposed two potential mechanisms that determine the response of the microstructure to geometric crowding.

In our work, we have presented a series of 2D full-melt-pool phase-field simulations, a series of multiscale simulations using a new line model approach, and an analysis of the error introduced by the assumptions in the multiscale model. We consider epitaxial solidification only and not nucleation in the liquid. The error in the multiscale model results is determined using quantities of interest that include measures of the solidification front (the cell/dendrite tip temperature and tip velocity) and the microstructure (primary arm spacing, secondary dendrite arm spacing, a hot cracking criterion, and the permeability). The contributions of this work are threefold:

- To our knowledge, this is the first systematic, quantitative comparison between the predictions of a full melt-pool phase-field simulation with multiple dendrite orientations/grains and a multiscale simulation involving a phase-field micromodel to assess the effects of the multiscale approximations. Our analysis demonstrates that the new line model yields similar values for most, but not all, of the quantities of interest as the full-melt-pool simulations. To identify the source of differences between these models, the analysis also includes a new model with assumptions between full melt-pool phase-field simulation and the line model.
- We present a new line model that associates every point in the melt pool with a single line model trajectory, permitting microstructure predictions at arbitrary locations.
- Our DNS simulations revealed a pattern that cannot be observed with existing steady-state point models or line models: a geometric crowding effect whereby the converging growth of the cells/dendrites tends to decrease the primary spacing unless the system can rapidly reorder to decrease the number of dendrites/cells.

3.2. Nonlocal phase-field models for solidification

Researchers: Olena Burkovska (ORNL), Stephen DeWitt (ORNL), Max Gunzburger (UT), Balasubramaniam Radhakrishnan (ORNL)

Phase-field approaches are commonly used for solidification modeling because they avoid having to explicitly track the interface [4]. Standard phase-field models have diffuse interfaces that result from a gradient energy term in the free energy functional that penalizes sharp changes in the solution and regularizes the solution at the interface to yield the physically expected interfacial energy. Whereas these

approaches have had significant success, the diffuse interface approach has an important drawback – the computational grid must be fine enough to have several points across the interface. For alloy solidification simulations in the additive manufacturing regime (rapid, directional solidification) this weakness is particularly apparent due to restrictions on the allowable interface thickness. These restrictions are a result of the breakdown of the assumptions in a part of the models known as the "anti-trapping current" as the diffusion length decreases below the interfacial thickness. Therefore simulations of the evolution of the solidification microstructure during additive manufacturing require very fine computational grids, with large computational costs, to resolve very thin interfaces relative to the microstructural feature sizes.

To address this problem, we are developing new solidification models with nonlocal interface formulations. Here we build upon previous work in AEOLUS, where a nonlocal Cahn-Hilliard model that can describe solutions with perfectly sharp interfaces was developed [7]. A nonlocal solidification phase-field model with sharp interfaces would sidestep the requirement to have multiple grid points across the interface and may provide a more robust alternative to the anti-trapping current as a way to prevent artifacts in the solution on computational grids scaled by the features of the solidification microstructure. Side-stepping the anti-trapping term will also allow us to incorporate non-equilibrium partitioning of solutes across rapidly moving solid-liquid interfaces observed in metallic alloys under AM solidification conditions. Our initial focus is on a nonlocal phase-field model of the solidification of a pure material. Here, typically a phase-field equation of Allen-Cahn type is coupled to a local diffusion equation describing the temperature evolution. We are interested in obtaining discontinuous solutions, which is the case for the nonlocal Allen-Cahn type problem only at steady state. In the transient phase, during interface motion, this model necessarily leads to diffuse interfaces. In light of this, we also derive a new non-mass conserving Cahn-Hilliard model to describe the interface evolution. This in essence "de-regularizes" the temporal derivative of the phase field variable from the space of square-integrable functions $L^2(\Omega)$ on the domain Ω to the dual space $H^{-1}(\Omega)$. This permits the solution to assume sharp interfaces during the whole time evolution and not only at the steady-state. We analyze the problem and derive well-posedness of time-discrete and continuous formulations, and regularity properties of the solution together with conditions under which sharp-interfaces are obtained [5].

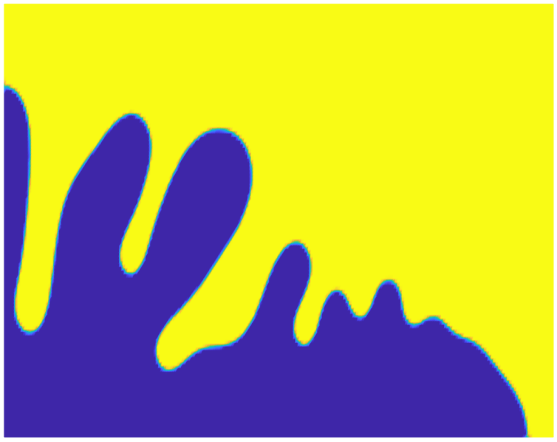


Figure 5: Simulation of nickel dendrite (isotropic) with nonlocal solidification model. The model is simulated on a coarse mesh and phase-field solution has sharp interfaces up to mesh resolution (∼1-2 cells).

Furthermore, in our ongoing work [6] we are evaluating the new model as an alternative to the established local models for solidification of pure materials, such as, e.g., [26, 31], in the context of relevant test cases and conducting a comparative study of the interface evolution. Here, our goals are threefold: (1) to demonstrate equivalence with a standard local model in the limit of a decreasing interfacial thickness (which has previously been demonstrated to be consistent with theory and observations), (2) to demonstrate improved accuracy on coarse computational grids compared to the local model, and (3) to lay the groundwork for a nonlocal, sharp interface phase-field model of alloy solidification.

4. Cross-cutting methods and broader applications

In contrast to the mathematical/computational/statistical advances in §2–§3, which have been tailored to driving advanced materials and manufacturing problems, we have made significant advances in cross-cutting research in inference, learning, optimization, optimal control, experimental design, uncertainty quantification, and model reduction methods that are applied more broadly. Ten of these are described

in §4.1–§4.10 below, while others are described in the publications listed in Appendix C.

4.1. Joint dimension reduction for Bayesian inference in non-Gaussian settings

Researchers: Ricardo Baptista (MIT), Michael Brennan (MIT), Youssef Marzouk (MIT)

Many dimension reduction methods for Bayesian inverse problems exploit the fact that the data inform only a low-dimensional subspace of the parameters, relative to the prior. Our past work has exploited such *likelihood-informed subspaces* [16, 30], and their extensions in the form of certified dimension reduction [17, 36], to accelerate many algorithms for Bayesian computation, ranging from Markov chain Monte Carlo [15] to Stein variational methods [11, 12].

A key idea underlying our recent work is that there exists a "dual" low-dimensional subspace of the data, which can be extracted and exploited in algorithms, with guarantees of optimal reduction in some cases and certified error bounds in others. In the past year, we have used this observation to create new methods for *joint reduction* of the parameters X and data Y for Bayesian inference. These methods are particularly useful for likelihood-free inference (LFI) algorithms, where the dimension of the data is otherwise a significant computational bottleneck. Let X_r denote coordinates in the retained low-dimensional subspace of the parameters, and $X_\perp$ coordinates in the complementary subspace; similarly, let Y_s describe the retained subspace of the data and $Y_\perp$ its complement. Then the expected error in the posterior can be bounded as $\mathbb{E}_Y[D_{KL}(\pi_{X|Y}||\widehat{\pi}_{X|Y})] = I(X,Y) - I(X_r,Y_s) \leq I(X_\perp, Y|X_r) + I(Y_\perp, X|Y_s)$. For distributions that satisfy a certain logarithmic Sobolev inequality (see details in [3, 36]), the conditional mutual information (CMI) terms on the right can themselves be bounded using averaged Hessian information. For example, the CMI between the parameters X and the "discarded" data $Y_\perp$ can be bounded as:

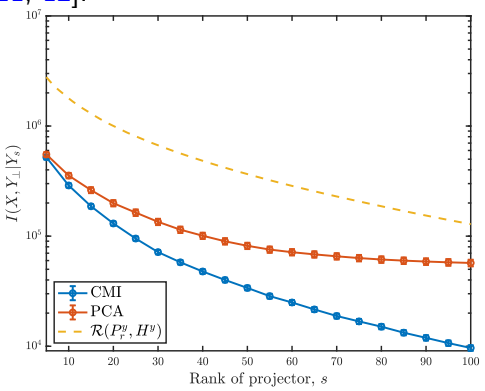


Figure 6: Posterior approximation error for different data projections.

$$I(X, Y_\perp|Y_r) \leq C_\pi \, \mathbb{E}_{\pi_{X,Y}} \|\nabla_x \nabla_{y_\perp} \log \pi(x,y)\|_F^2 = C_\pi \, \mathbb{E}_{\pi_{X,Y}} \|\nabla_x \nabla_{y_\perp} \log \pi(y|x)\|_F^2.$$

A similar expression applies for reduction of the parameters. These upper bounds can themselves be minimized over projectors of any given rank, yielding a joint dimension reduction method that controls posterior approximation error. Figure 6 illustrates results for a remote sensing inverse problem, where data projection based on our CMI bound performs significantly better than principal component analysis or even canonical correlation analysis. We have demonstrated initial versions of this reduction method in nonlinear filtering [27] and are currently evaluating its implications on performance and scaling of LFI methods in high dimensions.

4.2. Approximation and representation of transport maps

Researchers: Jakob Zech (MIT), Ricardo Baptista (MIT), Fengyi Li (MIT), Joshua Chen (UT), Youssef Marzouk (MIT)

Measure transport methods, which seek deterministic transformations between a simple/tractable "reference" probability measure and a more complex "target" probability distribution of interest, are central to many AEOLUS algorithmic developments and target applications. As detailed in earlier reports, these methods are useful for: (1) variational Bayesian inference, including certain optimization-based approaches to Bayesian inverse problems; (2) density estimation; (3) generative modeling; and (4) likelihood-free or simulation-based inference (as exemplified in our approach to parameter learning and optimal experimental design for phase separation of block copolymer melts [2] and reported on last year). Normalizing flows, now a standard tool in machine learning, are essentially specific parameterizations of

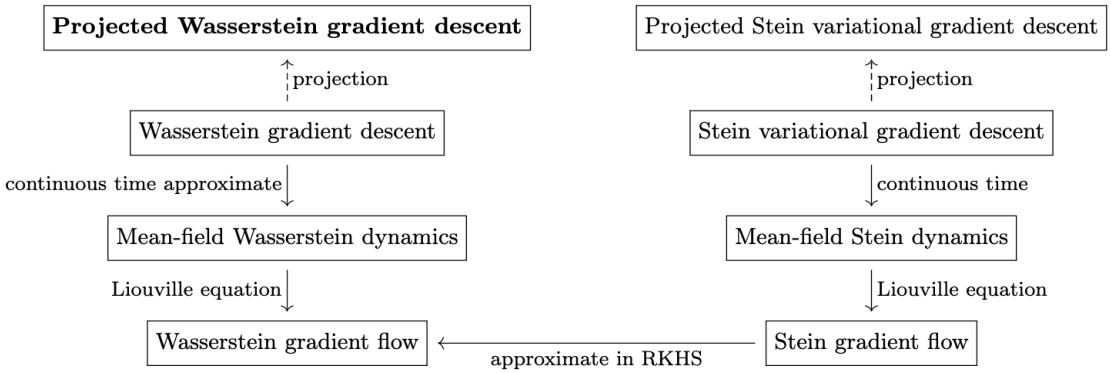


Figure 7: Relationship between pWGD, pSVGD, WGD, SVGD, and their corresponding dynamics and gradient flows.

transport maps, and the underlying transport ideas are closely related to both variational autoencoders and generative adversarial networks for generative modeling.

A key aspect of our AEOLUS effort has aimed at establishing a more fundamental understanding of the power and limitations of these techniques, and of their performance in high dimensions. To this end, we have recently published two papers [37, 38] that provide the first (to our knowledge) convergence analysis of parametric transport maps, focusing on sparse polynomial/rational approximations or ReLU neural network approximations of triangular maps on bounded domains. In the finite dimensional setting, specifically for probability measures ρ and π with analytic densities on the d-dimensional cube $[-1,1]^d$, we show that there exist approximations $\widetilde{T}$ of the triangular monotone Knothe–Rosenblatt rearrangement such that the distance between $\widetilde{T}_\sharp\rho$ and π converges exponentially fast. The notion of distance comprises the Hellinger distance, the total variation distance, the Wasserstein distance, and the Kullback–Leibler divergence. These rates do depend on dimension, however. In a second part of this effort, we have analyzed the infinite-dimensional setting, i.e., probability measures ρ and π on $[-1,1]^{\mathbb{N}}$. Here, under suitable assumptions, we show that the triangular Knothe–Rosenblatt map can be approximated by rational functions with a *dimension-independent* algebraic convergence rate. Our results are applicable to posterior measures arising in certain inference problems where the unknown belongs to an (infinite dimensional) Banach space. In particular, we show that it is possible to efficiently approximately sample from certain high-dimensional measures by transforming a lower-dimensional latent variable. In both the finite and infinite-dimensional settings, we give explicit *a priori* descriptions of anisotropic ansatz spaces that achieve the convergence rates described, useful for numerical implementations. Our ongoing work aims at addressing the case of unbounded domains, where precise control of the tails of transport maps (linked to the tails of the associated distributions) is a key challenge.

4.3. Wasserstein gradient flows for inverse problems

Researchers: Peng Chen (UT)

The Bayesian formulation of inverse problems is of central importance across such fields as machine learning, uncertainty quantification, and data assimilation. Sampling methods for high-dimensional Bayesian inference problems usually face the curse of dimensionality, i.e., the computational complexity grows rapidly (often exponentially) with parameter dimension. Following our recent work [12] on the projected Stein variational gradient descent (pSVGD) method, which demonstrates mitigation of the curse of dimensionality faced by SVGD, we proposed in [32] a projected Wasserstein gradient descent method (pWGD) and provided a detailed convergence analysis. (Figure 7 shows the relationships). Since WGD seeks a steepest descent direction in L^2 space for a transport map that minimizes the Kullback–Leibler divergence between the pushforward distribution and the posterior distribution at each iteration of the algorithm, and L^2 is bigger than the reproducing kernel Hilbert space (RKHS) used by

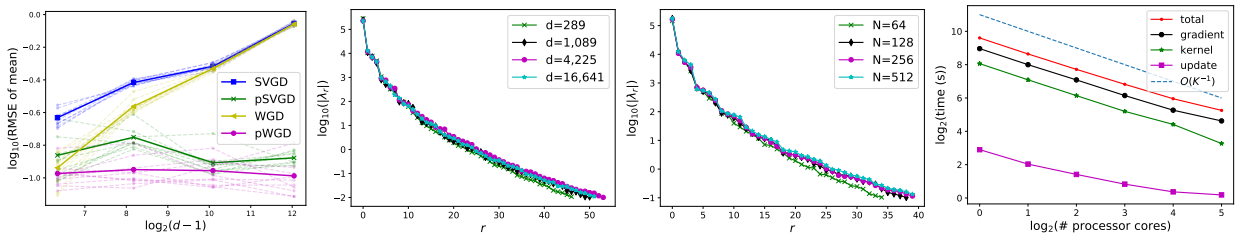


Figure 8: Left: pWGD preserves high accuracy with increasing dimension. Middle: Decay of the eigenvalues, indicating intrinsic dimensionality, is independent of parameter dimension and number of samples. Right: time vs CPU cores.

SVGD, we observe faster convergence of WGD relative to SVGD for low-dimensional inference problems, and faster convergence of pWGD relative to pSVGD for inference problems in high dimensions.

The underlying density function of a particle system of WGD is approximated by kernel density estimation (KDE), which is known to cause particle collapse in high dimensions. We overcome this challenge by exploiting the intrinsic low-dimensional structure of the difference between the posterior and prior distributions. The parameters are projected into a low-dimensional subspace to alleviate the approximation error of KDE in high dimensions. We formulated a projected Wasserstein gradient flow and analyzed its (exponential) convergence property under mild assumptions. Several numerical experiments illustrate the accuracy, convergence, and complexity scalability of pWGD with respect to parameter dimension, sample size, and processor cores (Figure 8). As an extension, we are currently working on using neural networks to approximate the Wasserstein gradient in high dimensions.

4.4. Advances in optimal experimental design

Researchers: Peng Chen (UT), Omar Ghattas (UT), Youssef Marzouk (MIT), Keyi Wu (UT)

Optimal experimental design (OED) is a principled framework for maximizing information gained from limited data in inverse problems, by optimizing the data acquisition (for example what to measure and when/where to measure it). Unfortunately, conventional methods for OED are prohibitive when applied to expensive models with high-dimensional parameters (as we target in AEOLUS), since the Bayesian inverse problem—by itself often intractable–must be solved at each iteration of OED. We extended our work [34] on a fast and scalable computational framework for large-scale and high-

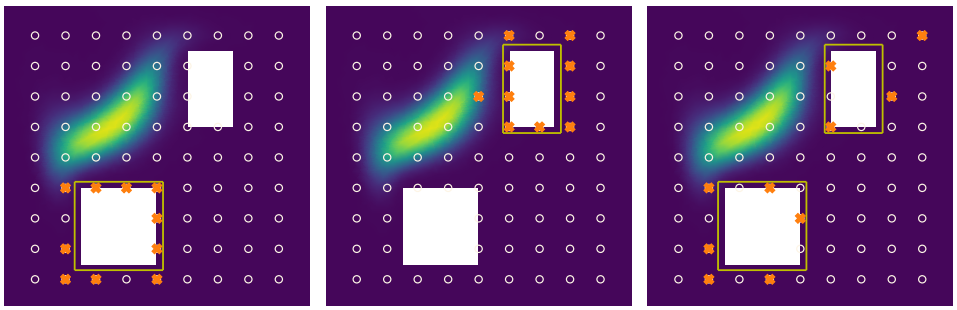


Figure 9: Sensors chosen by our fast method for goal-oriented Bayesian OED with three different prediction QoIs represented by the integral of the state along the boundary of the first, second, and both blocks.

dimensional nonlinear Bayesian OED (reported last year), and developed in [35] a fast and scalable computational framework for *goal-oriented* OED of large-scale Bayesian linear inverse problems that finds sensor locations to maximize the expected information gain (EIG) for a predicted quantity of interest (QoI) (Figure 9). By employing low-rank approximations of appropriate operators, an online-offline decomposition, and a new swapping greedy algorithm, we are able to maximize EIG at a cost measured in model solutions that is independent of the problem and sensor dimensions. We demonstrated the ef-

ficiency, accuracy, and both data- and parameter-dimension independence of the proposed algorithm for a contaminant transport inverse problem with infinite-dimensional parameter field. In ongoing work, we are developing a principled parsimonious neural network-based surrogate for the parameter-to-observable map to tackle the fully nonlinear Bayesian OED problem.

4.5. Optimization under uncertainty and chance-constrained optimization

Researchers: Peng Chen (UT) and Omar Ghattas (UT)

We developed a fast and scalable optimization method to solve chance-constrained optimization problems governed by PDEs with high-dimensional random parameters [13]. To address the critical computational challenges of expensive PDE solution and high-dimensional uncertainty, we constructed surrogates of the constraint function by Taylor approximation of the parameter-to-objective map. To tackle the difficulty of the nondifferentiability of the inequality chance constraint, we used a smooth approximation of the discontinuous indicator function involved in the chance constraint, and we applied a penalty method to transform the inequality constrained optimization problem to an unconstrained one. Moreover, we designed a gradient-based optimization scheme that gradually increases smoothing and penalty parameters to achieve convergence. Based on numerical experiments for a problem in optimal control of subsurface flows, we demonstrated the accuracy of the Taylor approximation, its ability to greatly accelerate constraint evaluations, the convergence of the continuation optimization scheme (Figure 10), and the scalability of the proposed method in terms of the number of PDE solves with increasing parameter dimension from $O(10^3)$ to $O(10^5)$.

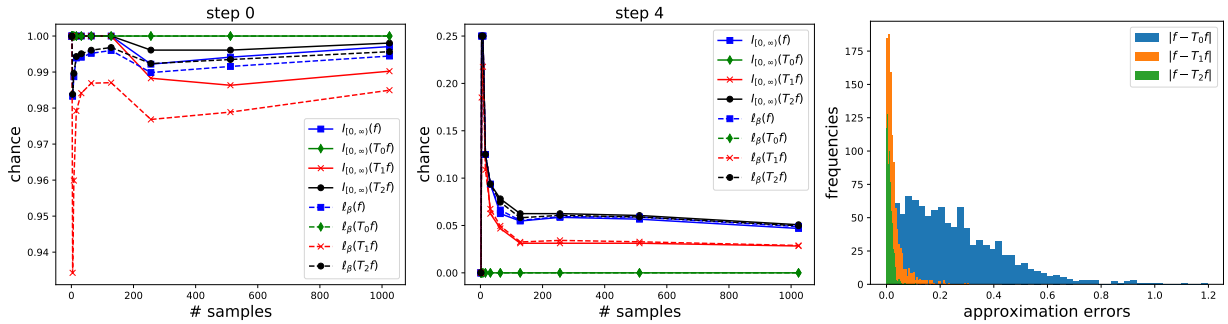
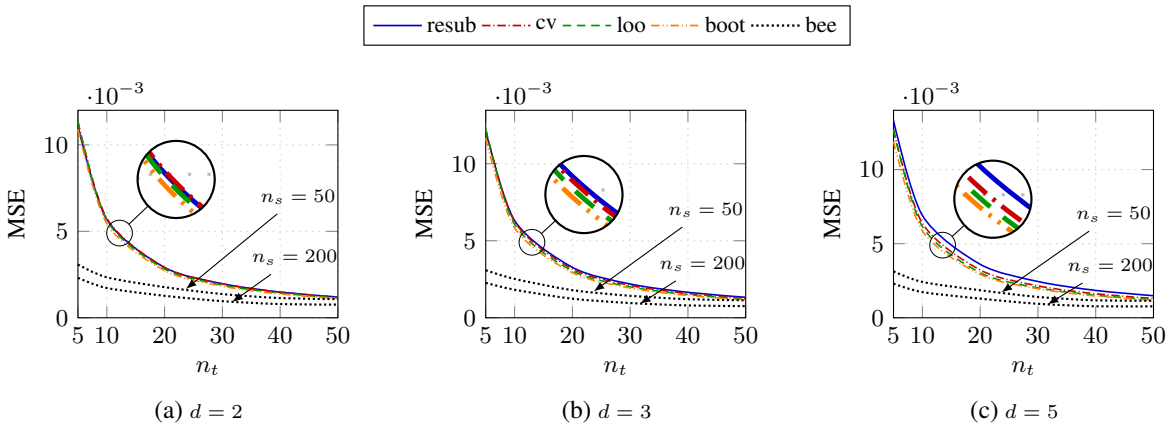


Figure 10: Left and middle: Chance constraint evaluated with different numbers of samples, by different Taylor approximations, and using different smoothing and penalty parameters at different steps (step 0 and 4). Right: Errors of different Taylor approximations.

Solutions of PDE-constrained optimization under uncertainty problems require various approximations, including finite-dimensional approximation of function-valued optimization variables, numerical approximation of PDE solutions, sample average approximation of risk measures or reliability constraints, smooth approximation of indicator functions involved in probability evaluation, and penalty approximation for statistical moments or probability constraints. In [14], we developed a general framework for a unified analysis of the impact of approximations on the system performance and established performance bounds for approximate solutions of optimization problems in various formulations. Specifically, under the convergence of each approximation, the performance or objective function at the cluster point of the approximate optimization solution can be bounded by the optimal solution up to an arbitrarily small positive constant. We demonstrated this analysis framework by applying it to a concrete example, a buffered probability-constrained optimal control problem. Based on this unified analysis, we are developing adaptive optimization algorithms to balance the approximation errors.

4.6. Non-intrusive model reduction for parameterized PDEs

Researchers: Parisa Khodabakhshi (UT), Shane McQuarrie (UT), Karen Willcox (UT)



(a) $d = 2$ (b) $d = 3$ (c) $d = 5$

Figure 11: MSE deviation from true error with respect to target data size. The proposed TL-based BEE is compared with other widely used estimators.

We developed a new framework for non-intrusive model reduction of parameterized time-dependent systems of PDEs. Our method embeds the affine parametric dependence into the reduced order model (ROM) by learning the corresponding ROM operators through a data-driven physics-based learning approach, *Parametric Operator Inference*. For non-affine parametric dependence, the desired affine structure can be approximated through the empirical interpolation method (EIM). The resulting parametric ROM can be evaluated for any value of the parameters without the need for interpolation between ROMs constructed for specific parameter values. The proposed formulation paves the way for parametric model reduction in high-dimensional parameter spaces with a reasonably small set of parameter samples in each parameter dimension. We have formulated a priori conditions—which are independent of the solution of the dynamical system—to be checked for the well-posedness of the learning scheme. In addition, a robust regularization scheme is introduced to guard against ill-conditioning and overfitting.

4.7. Optimal Bayesian transfer learning for error estimation

Researchers: Frank Alexander (BNL), Edward Doherty (TAMU), Xiaoning Qian (TAMU), Byung Jun Yoon (TAMU)

In many scientific or clinical settings, training data are typically limited, which impedes the design and evaluation of accurate classifiers. While transfer learning (TL) can improve the learning in the target domain by incorporating data from relevant source domains, it has received little attention for error estimation. In our recent work, we investigated the knowledge transferability in the context of error estimation within a Bayesian paradigm. We introduced a novel class of Bayesian minimum mean-square error (MMSE) estimators [18] for optimal Bayesian transfer learning (OBTL) [25], which enables rigorous evaluation of classification error under uncertainty in a small-sample setting. In our method, the relatedness between the target and source domains are mathematically represented through a joint prior of the model parameters, based on which useful knowledge and data can be transferred across domains. A key property of the proposed TL-based BEE is its inherent ability to handle the uncertainty about the model parameters in a Bayesian paradigm by integrating the prior with data, deducing robust estimates by accounting for all possible parameter values. Except for very simple cases, the error estimates based on the TL-based posterior probabilities cannot be analytically computed, and we proposed an efficient and robust importance sampling strategy that allows one to obtain TL-based Bayesian error estimates in practical applications.

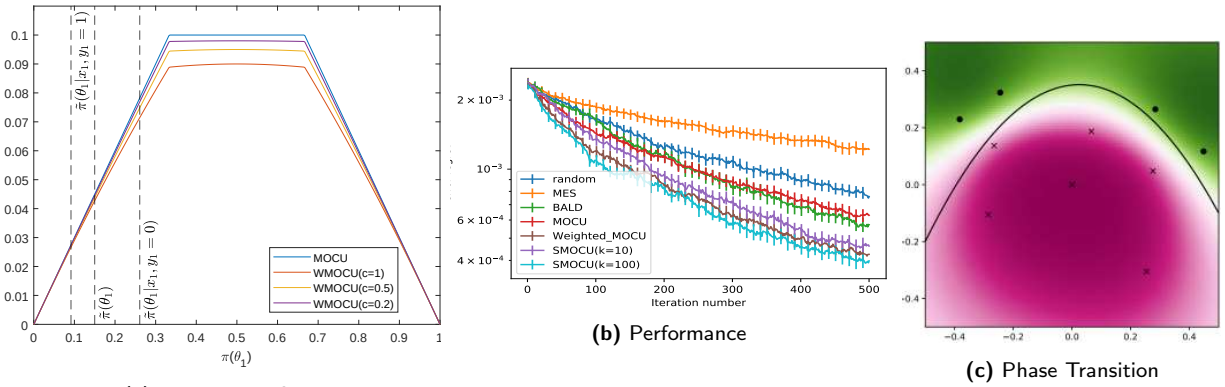
Through extensive experiments based on both synthetic data (e.g., see Figure 11) as well as real-world RNA sequencing (RNA-seq) data, we have investigated the performance of the proposed estimator for a

broad family of classifiers that span diverse learning capabilities. Experimental results have clearly shown that our proposed TL-based error estimation scheme clearly outperforms standard error estimators, especially in a small-sample setting, by tapping into the data from other relevant domains. Technical details of our method and further experimental results can be found in [28].

4.8. Active learning under model uncertainty

Researchers: Frank Alexander (BNL), Edward Doherty (TAMU), Xiaoning Qian (TAMU), Byung Jun Yoon (TAMU)

As collecting and labeling data is often expensive and highly time consuming, sample/label efficiency is one of the most important concerns in developing machine learning methods for scientific research and discoveries. Active learning is one strategy in machine learning that tries to address the problem and has been demonstrated for sample efficient learning with less required labeled data. In each active learning iteration, a candidate training sample is chosen for labeling by optimizing an acquisition function. Expected Loss Reduction (ELR) methods maximize the expected reduction in the prediction error given a new labeled candidate based on a one-step-look-ahead strategy. ELR is optimal considering a single query; however, it may get stuck before reaching the optimal model due to its myopic nature without considering the long-term effect of a query on the classification error. While these active learning methods based on one-step-look-ahead strategies are optimal, in terms of the maximum classification error reduction based on a single query, it is well-known that there is no performance guarantee in the long run for these myopic methods.



(a) Weighted MOCU **(b)** Performance **(c)** Phase Transition

Figure 12: (a) When the updated model posterior is not significant enough and the change is within the linear pieces, MOCU/ELR-based active learning may get stuck; (b) Comparison of different active learning methods based on the expected OBC error regret, demonstrating the effectiveness of Weighted- and Soft-MOCU based active learning methods; (c) The proposed active learning methods have the potential to help discover the phase transition diagram for materials systems of interest.

To improve convergence in the context of optimal Bayesian classification, we developed one-step-look-ahead acquisition functions based on a family of measures considering the mean objective cost of uncertainty (MOCU) that focuses on the uncertainty directly related to the classification error. Empirically, MOCU-based Bayesian active learning may still suffer from similar myopic behavior in the long run. We have analyzed its performance theoretically. To the best of our knowledge, we, for the first time in our work [41], discovered the piecewise linear structure of MOCU-based acquisition function with respect to the model posterior and identified the underlying reason for the observed myopic behavior (Figure 12a). We further proposed active learning based on a weighted form of MOCU. We proved that our proposed active learning algorithm converges to the optimal classifier of the true model. In [39], we proposed another strictly concave approximation of MOCU—referred as *Soft MOCU*—that can be

used to define an acquisition function to guide Bayesian active learning with the theoretical convergence guarantee. For training Bayesian classifiers with both synthetic and real-world data, our experiments demonstrated the superior performance of active learning by Soft MOCU compared to other existing methods (Figure 12b). Both papers have been published in the International Conference on Artificial Intelligence and Statistics (AISTATS) and the International Conference on Learning Representations (ICLR) this year.

We have recently started developing computationally efficient query synthesis active learning methods based on the Soft MOCU acquisition function, which enables efficient evaluation of continuous design space based on a new gradient estimator for Gaussian process classifiers (GPC). In particular, we have developed computationally efficient algorithms for Soft-MOCU based active learning with GPC. By deriving the joint predictive distribution of label pairs as a one-dimensional integral, the computation of the Soft-MOCU based acquisition function avoids retraining the GPC for each query, remarkably reducing the computational overhead. We have also derived the gradient chain rule to efficiently calculate the gradient of the acquisition function, which leads to the first query synthesis active learning algorithm implementing MOCU-based strategies. Such a computationally efficient algorithm is more suitable when exploring the continuous materials design space for example (Figure 12c). This work has been recently accepted in the 35th Conference on Neural Information Processing Systems (NeurIPS 2021) [40].

4.9. Optimal multiobjective/multifidelity computational campaign design

Researchers: Frank Alexander (BNL), Edward Doherty (TAMU), Xiaoning Qian (TAMU), Byung Jun Yoon (TAMU)

The need for effective selection of the potential molecular candidates (e.g., material compounds) that meet certain conditions based on desired target properties emerges in many real-world applications in various domains, including materials design and drug discovery. For example, since the Coronavirus disease 2019 (COVID-19) outbreak, an urgent scientific mission has been to screen known drug (or drug-like) small molecules to identify potential drugs that may effectively target the virus' spike proteins [29]. Such high-throughput virtual screening (HTVS) typically involves constructing a multi-stage pipeline that consists of various models with different fidelity and computational complexity. A typical pipeline places computationally cheaper models with lower fidelity at earlier stages to quickly filter out molecules that likely do not possess the desired properties. Complex higher-fidelity models are used in later stages for more accurate prediction of the molecular properties and accurate selection of candidates that meet the desired selection criteria. In real applications, such HTVS pipelines are often empirically constructed and operated, resulting in suboptimal performance.

In our recent work [33], we proposed an optimal decision-making framework for optimal computational campaign design. We considered two different scenarios, where in the first scenario, we aimed to design the optimal screening policy that can maximize the throughput of the pipeline given a finite computational budget. Next, we considered the problem of joint optimization of throughput and computational cost, where we aim to maximize the throughput while minimizing the overall cost of screening.

Figure 13: Optimal computational campaign for high-throughput virtual molecular screening.

Based on both synthetic as well as real examples, we have demonstrated that our proposed optimization framework significantly outperforms the baseline methods, in terms of efficiency, accuracy, and robustness. Figure 13 illustrates an example of a molecular screening pipeline that is constructed

by interconnecting several state-of-the-art lncRNA (long non-coding RNA) detection algorithms with different complexity and accuracy that was used for evaluating the HTVS optimization framework in a realistic setting. Experimental results show that optimal computational campaign based on our proposed method leads to up to 7-fold acceleration of the screening speed, with virtually no degradation in screening accuracy. Details of our proposed methods and the screening results can be found in [33]. We are currently applying the optimization framework to optimal screening of material compounds with desired reduction potential (redox potential), an important problem for advanced materials design for efficient batteries.

4.10. Nonlinear phase field models of vascular tumor growth

Researchers: Lianghao Cao (UT), David Fuentes (MDACC), Marvin Fritz (TUM), Prashant Jha (UT), Tobias Köppl (TUM), J. Tinsley Oden (UT), Andreas Wagner (TUM), Barbara Wohlmuth (TUM)

As an application of the multiscale modeling theory and algorithms developed within AEOLUS, we are continuing with our efforts in developing multi-species multiphase tumor growth models obtained as a generalization of the Cahn-Hilliard-type phase-field model employed in simulating phase separation in block copolymers (BCPs). At the mesoscale, tumor growth is a result of multiple constituents interacting with each other. Continuum mixture theory based on mechanistic principles serves as a framework to model the complex tumor growth phenomena. In our model, we consider multiple cell species, nutrients, and proteins released by hypoxic cancer cells and postulate appropriate Ginsburg-Landau free energy functionals and reaction terms to model the cancer growth. The free energy functional is similar to those in nonlocal Cahn-Hilliard models of BCP, except that it includes energetic contributions from various constituents.

Our focus also includes an accurate representation of vascular networks and thereby accurate vascular-interstitial flow; vasculature profoundly impacts the growth of tumor and drug therapy. Currently, we are developing a coupled multiscale vascular flow and tumor growth model in collaboration with colleagues at the Technical University of Munich; see Figure 14 where preliminary results using a multiscale vascular flow model are shown. In our model, the arteries, which can be segmented using magnetic resonance imaging (MRI) data, are retained as a discrete network, whereas capillaries are approximated by porous media. In addition, interstitial space is also modeled using porous media. This ongoing work extends our earlier work [20, 21, 23] where the vascular tumor growth model with discrete capillary flow was considered. We also note that parallel related work, e.g., [24], is continuing with colleagues at the MD Anderson Cancer Center (MDACC) in hopes of acquiring data for multiscale vascular tumor growth models of glioma. Here, the tumor growth model can simulate various treatment decisions and analyze the re-emergence of tumor post-treatment.

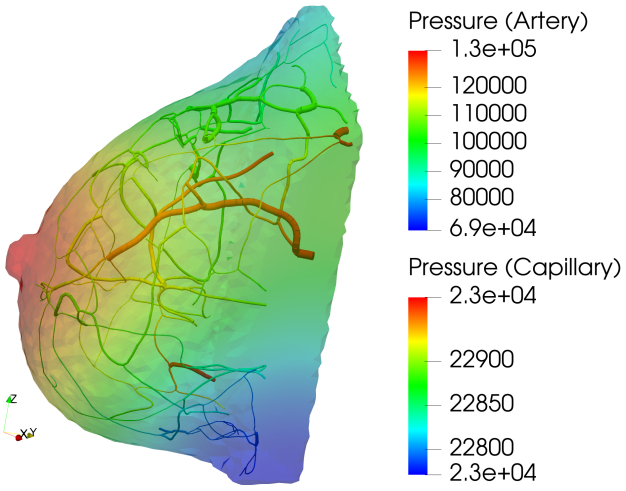


Figure 14: Simulation of flow within breast tissue using a multiscale 3D-1D flow model. Pressures in arterial network and homogenized capillary bed are shown.

References

[1] Yuanxun Bao, George Biros, Stephen DeWitt, Yigong Qin, and Balasubramaniam Radhakrishnan. Dendrite-resolved, full-melt-pool phase-field simulations to reveal non-steady-state effects and to test an approximate model. *Acta Materialia*, 2021. Submitted.

[2] Ricardo Baptista, Lianhao Cao, Joshua Chen, Omar Ghattas, Fengyi Li, Youssef Marzouk, and J. Tinsley Oden. Likelihood-free inference and information gain estimation from summary statistics: Adaptive Transport Maps for learning models from diblock copolymer images. *in preparation*, 2021.

[3] Ricardo Baptista, Youssef Marzouk, Rebecca E Morrison, and Olivier Zahm. Learning non-Gaussian graphical models via Hessian scores and triangular transport. *arXiv preprint arXiv:2101.03093*, 2021.

[4] W. J. Boettinger, J. A. Warren, C. Beckermann, and A. Karma. Phase-field simulation of solidification. *Annual Review of Materials Research*, 32(1):163–194, 2002.

[5] Olena Burkovska. Nonlocal phase-field models for solidification: analysis, sharp interfaces and discretization. In preparation, 2021.

[6] Olena Burkovska, Stephen DeWitt, Max Gunzburger, and Balasubramaniam Radhakrishnan. In preparation, 2021.

[7] Olena Burkovska and Max Gunzburger. On a nonlocal Cahn-Hilliard model permitting sharp interfaces. *Mathematical Models and Methods in Applied Sciences*, 31(09):1749–1786, 2021.

[8] Lianghao Cao, Daniil Bochkov, Omar Ghattas, and J. Tinsley Oden. A Hessian-free Newton method for solving the Self-Consistent Field Theory model for the self-assembly of diblock copolymer. In preparation (https://www.dropbox.com/s/uitxjloe9h1anxl/scft_newton.pdf?dl=0).

[9] Lianghao Cao, Omar Ghattas, and J. Tinsley Oden. A globally convergent modified Newton method for the direct minimization of the Ohta-Kawasaki energy with application to the directed self-assembly of diblock copolymers. *SIAM Journal on Scientific Computing*, 2022. To appear.

[10] Lianghao Cao and J. Tinsley Oden. On the derivation of the Self-Consistent Field Theory model for the self-assembly of diblock copolymers. In preparation (https://www.dropbox.com/s/6gegr374z3tykbv/examine_scft_paper.pdf?dl=0).

[11] P. Chen, K. Wu, J. Chen, T. O'Leary-Roseberry, and O. Ghattas. Projected Stein variational Newton: A fast and scalable Bayesian inference method in high dimensions. *NeurIPS*, 2019. https://arxiv.org/abs/1901.08659.

[12] Peng Chen and Omar Ghattas. Projected Stein variational gradient descent. In *Advances in Neural Information Processing Systems*, 2020.

[13] Peng Chen and Omar Ghattas. Taylor approximation for chance constrained optimization problems governed by partial differential equations with high-dimensional random parameters. *SIAM/ASA Journal on Uncertainty Quantification*, 9(4):1381–1410, 2021.

[14] Peng Chen and Johannes Royset. Performance bounds for PDE-constrained optimization under uncertainty. *arXiv preprint https://arxiv.org/submit/3986461*, 2021.

[15] Tiangang Cui, Kody JH Law, and Youssef M Marzouk. Dimension-independent likelihood-informed MCMC. *Journal of Computational Physics*, 304:109–137, 2016.

[16] Tiangang Cui, James Martin, Youssef M Marzouk, Antti Solonen, and Alessio Spantini. Likelihood-informed dimension reduction for nonlinear inverse problems. *Inverse Problems*, 30(11):114015, 2014.

[17] Tiangang Cui and Xin T Tong. A unified performance analysis of likelihood-informed subspace methods. *arXiv preprint arXiv:2101.02417*, 2021.

[18] Lori A Dalton and Edward R Dougherty. Bayesian minimum mean-square error estimation for classification error—part i: Definition and the bayesian mmse error estimator for discrete classification. *IEEE Transactions on Signal Processing*, 59(1):115–129, 2010.

[19] A. Dereventsov, C. G. Webster, and J. Daws. An adaptive stochastic gradient-free approach for high-dimensional blackbox optimization. In R. Twari, A. Mishra, N. Yada, and M. Pavone, editors, *Proceedings of International Conference on Computational Intelligence*, pages 333–348, Singapore, 2022. Springer Singapore.

[20] Marvin Fritz, Prashant K. Jha, Tobias Köppl, J. Tinsley Oden, Andreas Wagner, and Barbara Wohlmuth. Modeling and simulation of vascular tumors embedded in evolving capillary networks. *Computer Methods in Applied Mechanics and Engineering*, 384:113975, 2021.

[21] Marvin Fritz, Prashant K. Jha, Tobias Köppl, J. Tinsley Oden, and Barbara Wohlmuth. Analysis of a new multispecies tumor growth model coupling 3D phase-fields with a 1D vascular network. *Nonlinear Analysis: Real World Applications*, 61:103331, 2021.

[22] R. Geelen and K. Willcox. Localized non-intrusive reduced-order modeling in the operator inference framework. *Philosophical Transactions A, The Royal Society*, accepted for publication, 2021.

[23] David A. Hormuth, Caleb M. Phillips, Chengyue Wu, Ernesto A. B. F. Lima, Guillermo Lorenzo, Prashant K. Jha, Angela M. Jarrett, J. Tinsley Oden, and Thomas E. Yankeelov. Biologically-based mathematical modeling of tumor vasculature and angiogenesis via time-resolved imaging data. *Cancers*, 13(12), 2021.

[24] Prashant K. Jha, Christopher Walker, Reshmi Patel, Collin J. Harlen, Drew Mitchell, J. Tinsley Oden, Dawid Schellingerhout, Barbara Wohlmuth, James A. Bankson, and David Fuentes. Mutual-information based optimal data acquisition for hyperpolarized ^{13}c-pyruvate mri. *To be submitted*, 2021.

[25] Alireza Karbalayghareh, Xiaoning Qian, and Edward R Dougherty. Optimal bayesian transfer learning. *IEEE Transactions on Signal Processing*, 66(14):3724–3739, 2018.

[26] Ryo Kobayashi. Modeling and numerical simulations of dendritic crystal growth. *Physica D: Nonlinear Phenomena*, 63(3):410–423, 1993.

[27] Mathieu Le Provost, Ricardo Baptista, Youssef Marzouk, and Jeff Eldredge. A low-rank nonlinear ensemble filter for vortex models of aerodynamic flows. In *AIAA Scitech 2021 Forum*, page 1937, 2021.

[28] Omar Maddouri, Xiaoning Qian, Francis J Alexander, Edward R Dougherty, and Byung-Jun Yoon. Robust importance sampling for error estimation in the context of optimal bayesian transfer learning. *arXiv preprint arXiv:2109.02150*, 2021.

[29] Aymen Al Saadi, Dario Alfe, Yadu Babuji, Agastya Bhati, Ben Blaiszik, Alexander Brace, Thomas Brettin, Kyle Chard, Ryan Chard, Austin Clyde, et al. Impeccable: Integrated modeling pipeline for covid cure by assessing better leads. In *50th International Conference on Parallel Processing*, pages 1–12, 2021.

[30] Alessio Spantini, Antti Solonen, Tiangang Cui, James Martin, Luis Tenorio, and Youssef Marzouk. Optimal low-rank approximations of Bayesian linear inverse problems. *SIAM Journal on Scientific Computing*, 37(6):A2451–A2487, 2015.

[31] S.-L. Wang, R.F. Sekerka, A.A. Wheeler, B.T. Murray, S.R. Coriell, R.J. Braun, and G.B. McFadden. Thermodynamically-consistent phase-field models for solidification. *Physica D: Nonlinear Phenomena*, 69(1):189–200, 1993.

[32] Yifei Wang, Peng Chen, and Wuchen Li. Projected Wasserstein gradient descent for high-dimensional bayesian inference. *arXiv preprint arXiv:2102.06350*, 2021.

[33] Hyun-Myung Woo, Xiaoning Qian, Li Tan, Shantenu Jha, Francis J Alexander, Edward R Dougherty, and Byung-Jun Yoon. Optimal decision making in high-throughput virtual screening pipelines. *arXiv preprint arXiv:2109.11683*, 2021.

[34] Keyi Wu, Peng Chen, and Omar Ghattas. A fast and scalable computational framework for large-scale and high-dimensional Bayesian optimal experimental design. *arXiv preprint arXiv:2010.15196*, 2020.

[35] Keyi Wu, Peng Chen, and Omar Ghattas. A fast and scalable computational framework for goal-oriented linear Bayesian optimal experimental design: Application to optimal sensor placement. *arXiv preprint arXiv:2102.06627*, 2021.

[36] Olivier Zahm, Tiangang Cui, Kody Law, Alessio Spantini, and Youssef Marzouk. Certified dimension reduction in nonlinear Bayesian inverse problems. *arXiv:1807.03712*, 2021.

[37] J. Zech and Y. M. Marzouk. Sparse approximation of triangular transports. Part I: the finite dimensional case. *Constructive Approximation*, in press, 2021. arXiv:2006.06994.

[38] J. Zech and Y. M. Marzouk. Sparse approximation of triangular transports. Part II: the infinite dimensional case. *Constructive Approximation*, in press, 2021. arXiv:2107.13422.

[39] Guang Zhao, Edward R Dougherty, Byung-Jun Yoon, Francis J Alexander, and Xiaoning Qian. Bayesian active learning by soft mean objective cost of uncertainty. In *The 24th International Conference on Artificial Intelligence and Statistics (AISTATS 2021)*, 2021.

[40] Guang Zhao, Edward R Dougherty, Byung-Jun Yoon, Francis J Alexander, and Xiaoning Qian. Efficient active learning for Gaussian Process Classification by error reduction. In *The 35th Conference on Neural Information Processing Systems (NeurIPS 2021)*, 2021.

[41] Guang Zhao, Edward R Dougherty, Byung-Jun Yoon, Francis J Alexander, and Xiaoning Qian. Uncertainty-aware active learning for optimal Bayesian classifier. In *The 9th International Conference on Learning Representations (ICLR 2021)*, 2021.

A. Organizational chart

DRIVING SCIENTIFIC APPLICATION AREA: ADVANCED MANUFACTURING & MATERIALS	
additive manufacturing testbed (Restrepo)	materials self-assembly testbed (Alexander and Oden)
INTEGRATIVE RESEARCH THRUSTS	
Thrust 1: Learning predictive models via Bayesian inference & optimization (Webster & Willcox)	**Thrust 2: Optimizing** experiments, processes, & designs under uncertainty (Alexander & Ghattas)

RESEARCH SUB-THRUSTS							
large-scale Bayesian inference (Marzouk)	predictive multiscale models & inadequacy (Moser)	learning from scientific data (Webster)	low-dimensional & reduced modeling (Willcox)	multifidelity methods for OUU (Gunzburger)	large-scale Bayesian OED (Ghattas)	optimal operator design (Dougherty)	optimal control under uncertainty (Biros)

Table 1: AEOLUS organizational chart. Research is organized under two integrative research thrusts, each featuring four sub-thrusts that aim to overcome outer loop challenges in learning and optimization for complex uncertain models. Specific application to advanced manufacturing and materials systems will be carried out under two application testbeds.

B. Work breakdown

The following page lists all AEOLUS personnel during Year 3 of the center (October 2020–October 2021), their positions and institutional affiliations, and the percentage of their AEOLUS effort dedicated to each one of the major AEOLUS research tasks.

AEOLUS WORK BREAKDOWN STRUCTURE, YEAR 3 (October 2020 -- October 2021)

	Additive manufacturing	Materials self-assembly	Inference, inverse problems & learning from data	Low-dimensional modeling & reduced models	Optimization under uncertainty	Optimal experimental design	Predictive multiscale models & inadequacy	Administrative tasks	Total
George Biros, UT co-PI	45		10	30	10			5	100
Yuanxun Bao, UT postdoc	60		40	0	0				100
Yigong Qin, UT PhD student	50		0	50					100
Naveen Himthani, UT PhD student	0		100						100
Dhwanit Agarwal, UT PhD student							100		100
Omar Ghattas, UT PI and center co-director	5	10	15	15	15	15	5	20	100
Peng Chen, UT research associate		15	20	20	20	20	5		100
Nick Alger, UT postdoc			50	50					100
Amal Alghamdi, UT postdoc			50	50					100
Josh Chen, UT PhD student		25	50	25					100
Dingcheng Luo, UT PhD student		25		25	50				100
Tom O'Leary Roseberry, UT postdoc			40	30	30				100
Keyi Wu, UT PhD student			40	20		40			100
Robert Moser, UT co-PI			50				50		100
Todd Oliver, UT research scientist			50				50		100
Daniil Bochkov, UT postdoc		50					50		
J. Tinsley Oden, UT co-PI	10	40	5		15		30		100
Danial Faghihi, assistant professor, U. of Buffalo	25	20	10	5		25	15		100
Lianghao Cao, UT PhD student	10	70			20				100
Prashant Jha, UT research associate	10	70	10			10			100
Karen Willcox, UT PI and center co-director	10		20	40	10			20	100
Parisa Khodabakhshi, UT postdoc	30	20		50					100
Rudy Geelen, UT postdoc		30		70					100
Sean McBane, UT PhD student	10			50	40				100
Shane McQuarrie, UT PhD student			10	90					100
Youssef Marzouk, MIT PI		10	50			30		10	100
Ricardo Baptista, MIT PhD student		10	70	10		10			100
Kelvin Leung, MIT PhD student			100						
Fengyi Li, MIT PhD student						100			
Michael Brennan, MIT PhD student			100						
Francis Alexander, BNL PI		25	25			25	25		100
Gyorgy Matyasfalvi, BNL postdoc (now at Princeton)									
Anthony DeGennaro, BNL staff scientist		30		30		10	30		100
Vanessa Lopez-Marrero						100			
Nathan Urban BNL staff scientist						100			
Clayton Webster, UT/UTK PI		20	20	40	5	5		10	100
Max Gunzburger, UT Senior Researcher	30	20	10	30	10				100
Juan Restrepo, ORNL PI	100								100
Balasubramaniam Radhakrishnan, ORNL senior scientist	100								100
Olena Burkovska, Householder Fellow, ORNL	10	40	30	20					100
Stephen DeWitt, ORNL staff scientist	100								100
Edward Dougherty, TAMU PI			25	15	30	30			100
Xiaoning Qian, TAMU associate professor			25	25	25	25			100
Byung-Jun Yoon, TAMU associate professor			30	20	20	30			100
Omar Maddouri, TAMU PhD student			50		50				100
Mingzhou Fan, TAMU PhD student			50			50			100
Hyun-Myung Woo, TAMU PhD student				30	20	50			100

C. AEOLUS publications appeared or accepted, October 2020–October 2021

1. Adcock, B., Brugiapaglia, S., and Webster, C.G., Sparse polynomial approximation of high-dimensional functions, *SIAM Book Series in Computational Sciences and Engineering*, 2021.

2. Alger, N., Chen, P., and Ghattas O., Tensor train construction from tensor actions, with application to compression of large high order derivative tensors, *SIAM Journal on Scientific Computing*, 42(5):A3516–A3539, 2020.

3. Alghamdi, A., Hesse, M., Chen J., Villa, U., and Ghattas, O., Bayesian Poroelastic Aquifer Characterization from InSAR Surface Deformation Data. Part II: Quantifying the Uncertainty, *Water Resources Research*, 2021.

4. Ambartsumyan, I., Boukaram, W., Bui-Thanh, T., Ghattas, O., Keyes, D., Stadler, G., Turkiyyah, G., and Zampini, S., Hierarchical matrix approximations of Hessians arising in inverse problems governed by PDEs, *SIAM Journal on Scientific Computing*, 42(5):A3397–A3436, 2020.

5. Aretz, N., Chen, P., and Veroy, K., Sensor selection for hyper-parameterized linear Bayesian inverse problems. *PAMM*, Vol. 20(S1), pp. e202000357, 2021.

6. Benner, P., Goyal, P., Kramer, B., Peherstorfer, B., and Willcox, K., Operator inference for non-intrusive model reduction of systems with non-polynomial nonlinear terms. *Computer Methods in Applied Mechanics and Engineering*, Vol. 372, pp. 113433, December 2020.

7. Brunn, M., Himthani, N., Biros, G., Mehl, M., and Mang, A., CLAIRE: Constrained Large Deformation Diffeomorphic Image Registration on Parallel Computing Architectures, *Journal of Open Source Software*, 6 (61), June 2021

8. Brunn M., Himthani, N., Biros, G., Mehl, M., and Mang, A., Fast GPU 3D diffeomorphic image registration, *Journal of Parallel and Distributed Computing*, 149, 13pg, March 2021,

9. Brunn, M., Himthani, N., Biros, G., Mehl, M., and Mang, A., Multi-Node Multi-GPU Diffeomorphic Image Registration for Large-Scale Imaging Problems, *SC'20*, November 2020 (Atlanta, Virtual)

10. Boluki, S., Qian, X., and Dougherty, E., Optimal Bayesian supervised domain adaptation for RNA sequencing data, *Bioinformatics*, Vol. 37, No. 19, pp. 3212-3219, 2021.

11. Bukowski, R., Schulz, K., Gaither, K., Stephens, K.K., Semeraro, D., Drake, J., Smith, G., Cordola, C., Zariphopoulou, T., Hughes, T.J.R., Zarins, C., Kusnezov, D., Howard, D., and Oden, J.T. Computational medicine, present and the future: obstetrics and gynecology perspective, *American Journal of Obstetrics and Gynecology*, Vol. 224, No. 1, pp. 16-34, 2021.

12. Brennan, M., Bigoni, D., Zahm, O., Spantini, A., and Marzouk, Y.M, Greedy inference with structure-exploiting lazy maps. *Advances in Neural Information Processing Systems (NeurIPS)*, 2020.

13. Burkovska, O. and Gunzburger, M., On a nonlocal Cahn-Hilliard model permitting sharp interfaces, *Mathematical Models and Methods in Applied Sciences*, 1(9):1749–1786, 2021.

14. Burkovska, O., Glusa, C., and D'Elia, M., An optimization-based approach to parameter learning for fractional type nonlocal models, *Computers & Mathematics with Applications*, in press, 2021.

15. Cao, L., Ghattas, O., and Oden, J.T, A globally convergent modified Newton method for the direct minimization of the Ohta-Kawasaki energy with application to the directed self-assembly of diblock copolymers, arXiv: 2010.15271, to appear, *SIAM Journal on Scientific Computing*, 2021.

16. Chen, P. and Ghattas, O., Projected Stein variational gradient descent, *Advances in Neural Information Processing Systems 33 (NeurIPS 2020)*, December 2020.

17. Chen, P. and Ghattas, O., Taylor approximation for chance constrained optimization problems governed by partial differential equations with high-dimensional random parameters. *SIAM/ASA Journal on Uncertainty Quantification*, Vol. 9(4), pp.1381-1410, 2021.

18. Chen, P. and Ghattas, O., Stein variational reduced basis Bayesian inversion. *SIAM Journal on Scientific Computing*, Vol. 43(2), pp. A1163-A1193, 2021.

19. Chen, P., Haberman, M.R., and Ghattas, O., Optimal design of acoustic metamaterial cloaks under uncertainty. *Journal of Computational Physics*, Vol. 431, p.110114, 2021.

20. Chen, P., Wu, K., and Ghattas, O., Bayesian inference of heterogeneous epidemic models: Application to COVID-19 spread accounting for long-term care facilities. *Computer Methods in Applied Mechanics and Engineering*, Vol. 385, pp. 114020, 2021.

21. Chao, C., Reiz, S., Yu, C., Bungartz, H.J., and Biros, G., Fast Approximation of the Gauss-Newton Hessian Matrix for the Multilayer Perceptron, *SIAM Journal on Matrix Analysis and Applications*, 42 (1), 19pg, February 2021

22. Dereventsov, A., Webster, C.G., and Daws, J., An Adaptive Stochastic Gradient-Free Approach for High-Dimensional Blackbox Optimization, *Proceedings of International Conference on Computational Intelligence, Springer Singapore*, pp. 333-348, 2021.

23. Dereventsov, A., Petrosyan, A., and Webster, C.G., Greedy Shallow Networks: An Approach for Constructing and Training Neural Networks, *International Journal of Artificial Intelligence*, Vol. 2 (0974-0635), pp. 58-73, 2021.

24. Dexter, N., Tran, H., and Webster, C.G., On the Strong Convergence of Forward-Backward Splitting in Reconstructing Jointly Sparse Signals, *Set-Valued and Variational Analysis*, ISSN 1877-0533, pp. 1-15, 2021

25. Ehre, M., Papaioannou, I., Willcox, K., and Straub, D., Conditional reliability analysis in high dimensions based on controlled mixture importance sampling and information reuse. *Computer Methods in Applied Mechanics and Engineering*, Volume 381, August 2021, 113826.

26. Fritz, M., Jha, P.K., Köppl, T., Oden, J.T., Wagner, A., and Wohlmuth, B, Modeling and simulation of vascular tumors embedded in evolving capillary networks, *Computer Methods in Applied Mechanics and Engineering*, Vol. 384, pp. 113975, 2021.

27. Fritz, M., Jha, P.K., Köppl, T., Oden, J.T., and Wohlmuth, B., Analysis of a new multispecies tumor growth model coupling 3D phase-fields with a 1D vascular network, *Nonlinear Analysis: Real World Applications*, Vol. 61, pp. 103331, 2021.

28. Geelen, R. and Willcox, K, Localized non-intrusive reduced-order modeling in the operator inference framework, *Philosophical Transactions A*, The Royal Society, accepted for publication, 2021.

29. Ghattas, O. and Willcox, K., Learning physics-based models from data: Perspectives from inverse problems and model reduction. *Acta Numerica*, Vol. 30, pp. 445-554, 2021.

30. Hong, Y., Kwon, B., and Yoon, B.J., Optimal experimental design for uncertain systems based on coupled differential equations, *IEEE Access*, Vol. 9, pp. 53804-53810, 2021.

31. Hormuth, D.A., Phillips, C.M., Wu, C., Lima, E.A.B.F., Lorenzo, G., Jha, P.K., Jarrett, A.M., Oden, J.T., and Yankeelov, T.E, Biologically-Based Mathematical Modeling of Tumor Vasculature and Angiogenesis via Time-Resolved Imaging Data, *Cancers*, Vol. 13, No. 12, 2021.

32. Jagalur-Mohan, J., and Marzouk, Y.M, Batch greedy maximization of non-submodular functions: guarantees and applications to experimental design." *The Journal of Machine Learning Research*, in press (2021).

33. Kapteyn, M., Pretorius, J., and Willcox, K., A Probabilistic Graphical Model Foundation for Enabling Predictive Digital Twins at Scale. *Nature Computational Science*, Vol. 1, No. 5, May 2021, pp. 337-347.

34. Khodabakhshi, P., Willcox, K., and Gunzburger, M., A multifidelity method for a nonlocal diffusion model. *Applied Mathematics Letters*, Volume 121, November 2021, 107361.

35. Lorenzo, G., Hormuth, D.A., Jarrett, A.M., Lima, E.A. B. F., Subramanian, S., Biros, G., Oden, J.T., Hughes, T.J.R., and Yankeelov, T.E, Quantitative in vivo imaging to enable tumor forecasting and treatment optimization, arXiv: 2102.12602, 2021.

36. McBane, S. and Choi, Y, Component-wise reduced order model lattice-type structure design. *Computer Methods in Applied Mechanics and Engineering*, Vol. 381, 2021, p.113813.

37. McQuarrie, S., Huang, C. and Willcox, K., Data-driven reduced-order models via regularized operator inference for a single-injector combustion process. *Journal of the Royal Society of New Zealand*, Vol. 51, No. 2 pp. 194-211, 2021, DOI: 10.1080/03036758.2020.1863237.

38. O'Leary-Roseberry, T., Villa, U., Chen, P., and Ghattas, O., Derivative-informed projected neural networks for high-dimensional parametric maps governed by PDEs. *Computer Methods in Applied Mechanics and Engineering*, Vol. 388, pp.114199, 2021.

39. Portone, T. and Moser, R.D., Baysian inference of an uncertain generalized diffusion operator. *SIAM/ASA Journal on Uncertainty Quantification*, accepted for publication, 2021.

40. Reshniak, V. and Webster, C.G., Robust learning with implicit residual networks, *Machine Learning and Knowledge Extraction*, 3(1): 34-55, 2021.

41. Reshniak, V., Trageser, J., and Webster, C.G., A nonlocal feature-driven exemplar-based approach for image inpainting, *SIAM Journal on Imaging Sciences*, 13(4):2140-2168, 2020.

42. Subramanian, S., Scheufele, K., Himthani, N., and Biros, G., Multiatlas Calibration of Biophysical Brain Tumor Growth Models with Mass Effect, *23rd MICCAI*, October 2020 (Peru, Virtual)

43. Scheufele, K., Subramanian, S., and Biros, G., Fully Automatic Calibration of Tumor-Growth Models Using a Single mpMRI Scan, *IEEE Transactions on Medical Imaging*, September 2020

44. Tunc, B., Hormuth, D., Biros, G., and Yankeelov, T.E., Modeling of Glioma Growth with Mass Effect by Longitudinal Magnetic Resonance Imaging, *IEEE Transactions on Biomedical Engineering*, June, 2021

45. Uribe, F., Papaioannou, I., Marzouk, Y.M., and Straub, D., Cross-entropy based importance sampling with failure-informed dimension reduction for rare event simulation. *SIAM/ASA Journal on Uncertainty Quantification*, 9(2): 818–847 (2021).

46. Villa, U., Petra, N., and Ghattas, O., hIPPYlib: An Extensible Software Framework for Large-Scale Inverse Problems Governed by PDEs; Part I: Deterministic Inversion and Linearized Bayesian Inference, *ACM Transactions on Mathematical Software* 47(2):34, 2021.

47. Willcox, K., Ghattas, O., and Heimbach, P., The imperative of physics-based modeling and inverse theory in computational science, *Nature Computational Science*, Vol. 1, No. 3, pp. 166-168, 2021.

48. Xie, X., Bao, F., Maier, T., and Webster, C.G., Analytic continuation of noisy data using Adams Bashforth residual neural network, *Discrete & Continuous Dynamical Systems - S*, 1937-1179, 2021.

49. Xie, X., Webster, C.G., and Iliescu, T., Closure Learning for Nonlinear Model Reduction Using Deep Residual Neural Network, *Fluids*, 5(1,39):1-15, 2021.

50. Xu, Y., Narayan, A., Tran, H., and Webster, C.G., Analysis of the ratio of ℓ_1 and ℓ_2 norms in compressed sensing, *Applied and Computational Harmonic Analysis*, Vol 55, 486-511, 2021.

51. Yoon, B.J., Qian, X., and Dougherty, E., Quantifying the multi-objective cost of uncertainty, *IEEE Access*, Vol. 9, pp. 80351-80359, 2021.

52. Zech, J. and Marzouk, Y.M., Sparse approximation of triangular transports on bounded domains. Part I: the finite-dimensional case. *Constructive Approximation*, in press, 2021.

53. Zech, J. and Marzouk, Y.M., "Sparse approximation of triangular transports on bounded domains. Part II: the infinite-dimensional case." *Constructive Approximation*, in press, 2021.

54. Zhao, G., Dougherty, E.R., Yoon, B.J., Alexander, F.J., and Qian, X., Bayesian active learning by soft mean objective cost of uncertainty, *24th International Conference on Artificial Intelligence and Statistics (AISTATS 2021)*, 2021.

55. Zhao, G., Dougherty, E.R., Yoon, B.J., Alexander, F.J., and Qian, X., Efficient active learning for Gaussian Process Classification by error reduction, *35th Conference on Neural Information Processing Systems (NeurIPS 2021)*, 2021.

56. Zhao, G., Dougherty, E.R., Yoon, B.J., Alexander, F.J., and Qian, X., Uncertainty-aware active learning for optimal Bayesian classifier, *9th International Conference on Learning Representations (ICLR 2021)*, 2021.

D. AEOLUS invited presentations, October 2020–October 2021

D.1. Major keynote and plenary lectures at international conferences and other distinguished lectures

1. Ghattas, O. "Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems and optimal experimental design," *Opening Conference, NSF Institute for Mathematical and Statistical Innovation*, University of Chicago, October 7–9, 2020.

2. Ghattas, O. "Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems," *US National Congress on Computational Mechanics (USNCCM) 2021*, Chicago, July 2021.

3. Ghattas, O. "Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems," *MATHIAS 2021*, Paris, France, October 3–7, 2021.

4. Oden, J.T. "Phase field models of the growth of tumors embedded in an evolving vascular network: Dynamic 1D-3D models of angiogenesis." Invited Talk, VII Workshop on Mathematical and Computational Modeling of Tumor Growth, January 2021.

5. Oden, J.T. "An introduction to: The foundations of predictive computational science." Invited Talk, MDACC Data Science and Modeling Series, April 2021.

6. Webster, C., "Uncertainty quantification and approximation theory for parameterized PDEs," Invited short course, School of Mathematics, African Institute for Mathematical Sciences (AIMS), Cape Town, South Africa, November 2020.

7. Willcox, K. "Aerospace Design in the Age of Big Data and Big Compute." Invited Plenary Talk, AIAA SciTech Forum & Exhibition, January 2021.

8. Willcox, K. "A Probabilistic Graphical Model Foundation for Predictive Digital Twins." Invited Plenary Talk, SIAM Conference on Computational Science and Engineering, March 2021.

9. Willcox, K. "Predictive Digital Twins and the Data-driven Future of Computational Science." Invited Keynote Talk, AI CON, March 2021.

10. Willcox, K. "Predictive Digital Twins: From physics-based modeling to scientific machine learning." Invited Keynote Lecture, CAASE21, June 2021.

11. Willcox, K. "A Probabilistic Graphical Model Foundation for Enabling Predictive Digital Twins at Scale," Invited Plenary Lecture, European Control Conference, July 2021.

12. Willcox, K. "Predictive Digital Twins: From physics-based modeling to scientific machine learning." *Opening Conference, NSF Institute for Mathematical and Statistical Innovation*, University of Chicago, October 7–9, 2020.

13. Willcox, K. "Predictive Digital Twins and the Data-Driven Future of Aerospace Systems." Invited Keynote Talk, the 13th International Symposium on Non-Destructive Testing (NDT) in Aerospace, NASA Langley Research Center, October 2021.

14. Willcox, K. "Engineering Design in the Age of Big Data and Big Compute." Invited Plenary Talk, NAFEMS World Congress, October 2021.

D.2. Other invited conference and workshop talks

15. Agarwal, D., Biros, G., "Novel Algorithms for 3D Deformable Capsules Simulations", Minisymposium on Recent Advances in Fast Algorithms and Discretization Techniques for Integral Equations, SIAM Conference on Computational Science and Engineering, Virtual, March 2021

16. Biros, G., "Scalable algorithms for diffeomorphic image registration", Workshop on "Inverse Problems and Optimization", University College London, Virtual, May 6, 2021

17. Biros G., "Inverse biophysical modeling and its application to neurooncology", Frontiers in Applied Mathematics and Computation, Harvard University, Virtual, April 2021

18. Chen, C., Biros, G., "A Fast Solver for Integral Equations using Domain Decomposition", Minisymposium on Fast Kernel Methods for Integral Equations, SIAM Conference on Computational Science and Engineering, Virtual, March 2021

19. Burkovska, O. "An optimization-based approach to parameter learning for truncated fractional models." Invited Talk, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology Conference, September, 2021.

20. Burkovska, O. "Identifying the parameters in nonlocal models related to the integral fractional Laplacian." Invited Talk, IFIP TC7 Conference on System Modelling and Optimization, September, 2021.

21. Burkovska, O. "Nonlocal phase-field models for describing sharp interface dynamic." Invited Talk, 16th US National Congress on Computational Mechanics, July, 2021.

22. Burkovska, O. "Phase-field models with nonlocal interactions in the context of solidification." Invited Talk, IX International Conference on Coupled Problems in Science and Engineering, June, 2021.

23. Burkovska, O. "Nonlocal phase-field models permitting sharp interfaces." Invited Talk, SIAM Conference on the Mathematical Aspects of Materials Science, May, 2021.

24. Burkovska, O. "Nonlocal phase-field models permitting sharp interfaces." Invited Talk, 50th Barrett Memorial Lectures, Approximation, Applications, and Analysis of Nonlinear Nonlocal Models, University of Tennessee, May, 2021.

25. Burkovska, O. "An optimization-based approach to parameter learning for truncated fractional models." Invited Talk, SIAM Conference on Computational Science & Engineering, March, 2021.

26. Burkovska, O. "Nonlocal operators in phase-field models." Invited Seminar Talk, University of Nebraska-Lincoln, October, 2020.

27. Chen, P. "Stein Variational Reduced Basis Bayesian Inversion." Invited Talk, SIAM Annual Meeting, July, 2021.

28. Chen, P. "Fast and scalable computational methods for learning and optimization under uncertainty." Invited Talk, Xi'an Jiaotong University, May, 2021.

29. Chen, P. "Projected Variational Methods for High-dimensional Bayesian Inference." Invited Talk, Cornell University, April, 2021.

30. Chen, P. "Taylor Approximation for Chance Constrained Optimization." Invited Talk, SIAM Conference on Computational Science & Engineering, March, 2021.

31. Chen, P. "Taylor approximation for PDE and chance constrained optimization under uncertainty." Invited Talk, Banff Workshop on optimization under Uncertainty: Learning and Decision Making, February, 2021.

32. Chen, P. "Break the curse of dimensionality of Bayesian inference by projected variational transport methods, with application in COVID-19." Invited Talk, University of California, Los Angeles, September, 2020.

33. DeWitt, S. "Preparing for Exascale Phase-Field Simulation: Phase-Field Modeling in ExaAM and AEOLUS", Invited Talk, CHiMaD Phase-Field Methods Workshop XI, May 2021.

34. Geelen, R., Willcox, K. "Localized non-intrusive reduced-order modeling in the operator inference framework." 16th U.S. National Congress on Computational Mechanics (USNCCM16), July 2021.

35. Geelen, R., Willcox, K. "Localized non-intrusive reduced-order modeling in the operator inference framework." Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET 2021), September 2021.

36. Ghafouri, A., Biros, G.,, "Anisotropic Tau-Protein Spreading Model in Alzheimer's Disease from PET-MRI", Minisumposium on Biological Model Development and Data in Parallel, SIAM Conference on Computational Science and Engineering, Virtual, March 2021

37. Ghattas, O., Derivative-informed projected neural networks for high-dimensional parametric maps governed by PDEs, *RICAM Hybrid Prequel Workshop on Tomography Across the Scales*, Johann Radon Institute (RICAM), Austrian Academy of Sciences, Linz, Austria, October 15, 2021.

38. Ghattas, O., Integration of large-scale data and complex models via Bayesian inversion and HPC, *Building Community @ UT for a New Era in Astrophysics*, virtual, May 24–26, 2021.

39. Ghattas, O., Parsimonious structure-exploiting deep neural network surrogates for parameter-to-output maps governed by PDEs, *ARPA-E DIFFERENTIATE Program Workshop on Generative Models*, online, April 15, 2021.

40. Ghattas, O., Scalable Structure-Exploiting Approaches to Optimal Experimental Design, *SIAM Conference on Computational Science & Engineering*, online, March 1–5, 2021.

41. Ghattas, O., Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems, *Robert J. Melosh Medal Competition for Best Student Paper in Finite Elements*, Duke University, Durham, NC, October 22–23, 2020. (Online)

42. Ghattas, O., Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems, *Society for Engineering Science, 2020 Virtual Technical Meeting*, September 29–October 1, 2020.

43. Ghattas, O., Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems, *Colloquium*, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, July 1, 2021.

44. Ghattas, O., Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems, *GFDL Seminar Series*, Geophysical Fluid Dynamics Laboratory, Princeton, NJ, May 6, 2021.

45. Ghattas, O., Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems, *MOX Colloquia*, Modeling and Scientific Computing Lab, Department of Mathematics, Politecnico di Milano, Italy, November 12, 2020.

46. Ghattas, O., Large-scale PDE-constrained stochastic optimization, *Operations Research & Industrial Engineering Seminar Series*, The University of Texas at Austin, October 16, 2020.

47. Himthani, N., Biros, G., "Mass Effect Quantification through Image Registration", Minisymposium on Computational Modeling of Uncertainty in Biomedical Simulations, SIAM Conference on Computational Science and Engineering, Virtual, March 2021

48. Khodabakhshi, P., Gunzburger, M., Willcox, K., Multifidelity methods for uncertainty quantification of nonlocal diffusion model, 16th U.S. National Congress on Computational Mechanics (USNCCM16), July 2021.

49. Khodabakhshi, P., Willcox, K., Data-driven reduced order modeling for solidification processes in additive manufacturing, SIAM Conference on Computational Science and Engineering (CSE21), March 2021.

50. Khodabakhshi, P., Willcox, K., Structure-exploiting nonlinear model reduction with application to solidification of metals, 14th Word Congress in Computational Mechanics (WCCM), January 2021.

51. Marzouk, Y., NASA Jet Propulsion Laboratory. Pasadena, CA (virtual). October 2020.

52. Marzouk, Y. Dartmouth College, Department of Mathematics, Sea Ice Modeling and Data Assimilation seminar. Hanover, NH (virtual). October 2020.

53. Marzouk, Y., ExxonMobil, Applied Geophysics Research Seminar. Spring, TX (virtual). November 2020.

54. Marzouk, Y., MIT Technology Review, Future Compute 2021. Featured speaker. Cambridge, MA (virtual). February 2021.

55. Marzouk, Y., "Workshop on Optimization under Uncertainty: Learning and Decision Making." Banff International Research Station. Banff, Canada (virtual). February 2021.

56. Marzouk, Y., Courant Institute for Mathematical Sciences (NYU), Numerical Analysis and Scientific Computing Seminar. New York, NY (virtual). February 2021.

57. Marzouk, Y., SIAM Conference on Computational Science and Engineering. Fort Worth, TX (virtual). March 2021.

58. Marzouk, Y., University of Massachusetts, Amherst; Applied Mathematics and Computation Seminar. Amherst, MA (virtual). March 2021.

59. Marzouk, Y., University of Iowa, Numerical Analysis Seminar. Iowa City, IA (virtual). March 2021.

60. Marzouk, Y., Yale University, Applied Mathematics Seminar. New Haven, CT (virtual). April 2021.

61. Marzouk, Y., SIAM Conference on Mathematical and Computational Issues in the Geosciences. Milan, Italy (virtual). June 2021.

62. Marzouk, Y., Pacific Earthquake Engineering Research Center (PEER) International Forum. Berkeley, CA (virtual). June 2021.

63. Marzouk, Y., SIAM Annual Meeting (AN21). Invited minisymposium (virtual). July 2021.

64. Marzouk, Y., Bernoulli-IMS 10th World Congress on Probability and Statistics. Invited session speaker. Seoul, Korea. July 2021.

65. Marzouk, Y., Bath-ICMS workshop on "Analytical and Geometric Approaches to Machine Learning." Invited speaker. Bath, United Kingdon (virtual). July 2021.

66. Marzouk, Y., RWTH Aachen University, Chair of Mathematics for Uncertainty Quantification, Seminar. Aachen, Germany (virtual). July 2021.

67. Marzouk, Y., University of Potsdam. SFB 1294 kickoff meeeting (keynote). Potsdam, Germany (virtual). September 2021.

68. Marzouk, Y., CERN, Seminar on Machine Learning for Simulation. Geneva, Switzerland (virtual). September 2021.

69. Marzouk, Y., Centre International de Rencontres Mathematiques (CIRM) workshop, "On future synergies for stochastic and learning algorithms." Marseille, France (virtual). September 2021.

70. Marzouk, Y., George Washington University, Center for Mathematics and Artificial Intelligence (CMAI) Colloquium (virtual). October 2021.

71. McBane, S., "Accelerated topology optimization of lattice structures using component-wise reduced order modeling." SIAM Conference on Computational Science and Engineering, invited minisymposium presentation, March 2021.

72. McQuarrie, S., Huang, C., Willcox, K. "Data-driven reduced-order models via regularized operator inference." SIAM Conference on Computational Science and Engineering 2021 (CSE21), March 2021.

73. McQuarrie, S., Huang, C., Willcox, K. "Data-driven reduced-order models via regularized operator inference for a single-injector combustion process." SIAM Conference on Control and Its Applications 2021 (CT21), July 2021.

74. McQuarrie, S., Khodabakhshi, P., Willcox, K. "Non-intrusive parametric reduced-order modeling via operator inference." 16th U.S. National Congress on Computational Mechanics (USNCCM16), 28 July 2021

75. Qian, X. "Bayesian Active Learning by Objective-Oriented Uncertainty Quantification", Invited Talk, International Workshop on Signal and Information Intelligent Learning & Processing (SIILP), July 2021.

76. Qin, Y., Biros, G., "Multiscale Modeling in Additive Manufacturing and Reduced-Order Models", Minisymposium on Multiscale Simulations for Manufacturing and Materials Synthesis, SIAM Conference on Computational Science and Engineering, Virtual, March 2021

77. Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, University of Pennsylvania, October 2020.

78. Subramanian, S., Biros, G., "An Inverse Solver with Sparse Localization for Tumor Growth Models", Minisymposium on Computational Methods for Inverse Problems, SIAM Conference on Computational Science and Engineering, Virtual, March 2021

79. Webster, C., "Sparsity-enforced regularizations for optimal learning of high-dimensional systems from random sampling," Babuska Forum Lecture, Oden Institute for Engineering and Computational Sciences, The University of Texas at Austin, April 2021.

80. Webster, C., "An Adaptive Stochastic Gradient-Free Approach for High-Dimensional Blackbox Optimization," Workshop on Scientific Computing and Applications, The University of Las Vegas, Las Vegas, NV, July 2021.

81. Webster, C., "An Adaptive Stochastic Gradient-Free Approach for High-Dimensional Blackbox Optimization," The Fields Instittue, The University of Toronto, Toronto, ON, August 2021.

82. Webster, C., "Robust learning with implicit residual networks," Safety and Security of Deep Learning (Virtual), Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University, Providence, RI, 2021.

83. Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, University of Pennsylvania, October 2020.

84. Willcox, K. Invited Panelist, Mathematical Foundations Panel. Sandia National Laboratories Trusted AI Roundtable, October 2020.

85. Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, Texas A&M University, October 2020.

86. 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.

87. Willcox, K. "Digital Twins and Their Applications." Workshop on Digital Twins in Production Engineering and High Performance Computing Education, Invited Plenary Talk, U. Tennessee, December 2020.

88. Willcox, K. "The future needs Computational Science and Engineering." Invited Talk at Technology Convergence for a Smarter, More Connected World: Market Trends, CIMdata Community Webinar, December 2020.

89. Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." ECE Distinguished Lecture at George Washington University, December 2020.

90. Willcox, K. "Research and Education at the Oden Institute for Computational Engineering and Science." Invited Talk, MD Anderson Cancer Center, December 2020.

91. Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk at Workshop on Machine Learning for Engineering Modeling, Simulation, and Design. Neural Information Processing Systems (NeurIPS), December 2020.

92. Willcox, K. "Big Data, Big Models and Digital Twins: Computational Perspectives from Aerospace Engineering" Invited Keynote Talk, DOE/NCI Workshop on Accelerating Precision Radiation Oncology through Advanced Computing and Artificial Intelligence, January 2021.

93. Willcox, K. "Predictive Digital Twins for engineering systems: From physics-based modeling to scientific machine learning." Invited Talk, Christ's College Engineering Society, University of Cambridge, March 2021.

94. Willcox, K. "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, Sayas Numerics Seminar, April 2021.

95. Willcox, K. "Predictive Digital Twins and the Data-driven Future of Computational Science." Invited Talk, Indian Institute of Science, April 2021.

96. Willcox, K. "Predictive Digital Twins and the Data-driven Future of Computational Science." Invited Talk, College of Engineering Distinguished Lecture Series, New Mexico State University, April 2021.

97. Willcox, K., "Operator Inference: Bridging Model Reduction and Scientific Machine Learning." Invited Talk, Computational Mathematics and Applications Seminar, Oxford University, May 2021.

98. Willcox, K. "Transformational Technology Approaches for Dynamic Statistical, Data-Driven, and Mechanistic Modeling," Keynote Lecture, NCI Joint VIRTUAL Project Teams Meeting: Cancer Biology Machine Learning/Mechanistic Modeling and Cancer Patient Digital Twin, July 2021.

99. Willcox, K. "Digital Twins for Complex Engineering Systems: From Physics Based Models to Scientific Machine Learning," ISA/SPE Digital Transformation Virtual Conference (Invited), August 2021.

100. Willcox, K. "A Probabilistic Graphical Model Foundation for Enabling Predictive Digital Twins at Scale," RTRC Fellows Lecture (Invited), Raytheon Technologies Corporation, August 2021.

101. Willcox, K. "Predictive Digital Twins: Mathematical Foundations and Application to Structural Health Monitoring," Keynote Lecture, MaP Scientific Symposium, ETH Zurich, August 2021.

102. Willcox, K. "Predictive Digital Twins: Perspectives from Aerospace Engineering." Invited Talk, Data Science Work Group, MD Anderson Cancer Center, August 2021.

103. Willcox, K. "Predictive Digital Twins: From physics-based modeling to scientific machine learning." Invited Keynote Talk, Computing in Engineering Forum, University of Wisconsin-Madison, September 2021.

104. Willcox, K. "Research needs and future directions: Scaling digital twins from the artisanal to the industrial." Invited Plenary Talk, Workshop on Aviation Digital Twins: Applications and Opportunities, the MITRE Corporation, October 2021.

105. Willcox, K. "Mathematical and Computational Foundations for Enabling Predictive Digital Twins at Scale." Invited Talk, Santa Fe Institute, October 2021.

106. Willcox, K. "Predictive Digital Twins." Invited Talk, MD Anderson Cancer Center Data Science and Modeling Forum, October 2021.

107. Zhao, G., Dougherty, E., Yoon, B.J., Alexander F., and Qian, X., "Bayesian Active Learning by Soft Mean Objective Cost of Uncertainty", the 24th International Conference on Artificial Intelligence and Statistics (AISTATS), April 2021.

108. Zhao, G., Dougherty, E., Yoon, B.J., Alexander F., and Qian, X., "Uncertainty-aware Active Learning for Optimal Bayesian Classifier," the 9th International Conference on Learning Representations (ICLR), May 2021.

E. Other significant dissemination

Besides the traditional avenues for dissemination of research (publications and presentations), the AEOLUS team has been actively sharing the results of its research with the broader scientific community via other mechanisms, including public software releases, teaching of summer schools and short courses, development of new semester-long courses, co-organization of topical workshops and conference, and training of Ph.D. students and postdocs who move on to academic, laboratory, and industry positions.

E.1. Software

- GOFMM (Geometry Oblivious Fast Multipole method) is an algorithm for compressing kernel matrices in arbitrary dimensions. GOFMM can also compress arbitrary symmetric positive definite matrices. GOFMM supports shared and distributed memory parallelism. To our knowledge GOFMM is the only open source software with such capabilities.
https://github.com/ChenhanYu/hmlp

- hIPPYlib: Inverse Problem PYthon library. hIPPYlib implements state-of-the-art scalable adjoint-based algorithms for PDE-based deterministic and Bayesian inverse problems. It builds on FEniCS for the discretization of the PDE and on PETSc for scalable and efficient linear algebra operations and solvers.
https://hippylib.github.io/

- KNN-DBSCAN is a shared and distributed memory parallel library for linkage-based point clustering in high-dimensions. Unlike the original DBSCAN which uses range search nearest neighbors, KNN-DBSCAN uses approximate k-nearest neighbors and results in better scalability.
https://github.com/ut-padas/knndbscan

- Matlab code for robust filtering and OED with stochastic differential equations (SDEs):
https://github.com/QianLab/SDE-MOCU

- MIT TransportMaps library:
http://transportmaps.mit.edu

- MUQ: MIT Uncertainty Quantification Library:
http://muq.mit.edu

- OK Newton: Numerical implementation of a fast, globally convergent modified Newton method for the direct minimization of the Ohta-Kawasaki energy.
https://lcao11@bitbucket.org/lcao11/ok_newton/src/master/

- Operator Inference model reduction package with tutorial examples. Released June 2020.
https://github.com/Willcox-Research-Group/rom-operator-inference-Python3

- Python code for active learning with Soft MOCU based acquisition function:
https://github.com/QianLab/Soft_MOCU

- Python code for active learning with Weighted MOCU based acquisition function:
https://github.com/QianLab/WMOCU_AL

- Python code for Bayesian supervised domain adaptation:
https://github.com/SHBLK/BSDA

- Python code for Kuramoto model OED (optimal experimental design) simulations in GitHub:
https://github.com/yhong2/Sync

E.2. Short courses/summer schools taught and long courses developed

- Qian, X., Short courses on introductory machine learning in the iDiscovery Workshop on Data Science Foundations and Computational Practice, Texas A&M Institute of Data Science, May 2021.

E.3. Workshops and conferences co-organized

Team members served as co-chairs or co-organizers of the following workshops and conferences on AEOLUS-related themes.

- Alexander and Ghattas are on the Program Committee for the New York Scientific Data Summit 2021, October 26–29, 2021. https://www.bnl.gov/nysds21/
- Ghattas and Marzouk are co-organizing the Workshop on Mathematical Foundations of Data Assimilation and Inverse Problems at the Foundations of Computational Mathematics (FoCM'23) Conference in Whistler, Canada, June 12-21, 2023.
- Marzouk was co-chair of the SIAM Conference on Mathematical and Computational Issues in the Geosciences (GS21), held virtually in June 2021.
- Webster was a co-organizer of the Workshop on Safety and Security of Deep Learning, held virtually at the Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University, Providence, RI, April 2021
- Willcox is a co-chair of the SIAM Conference on Mathematics for Data Science (MDS22), to be held September 2022.
- Willcox serves on the Organizing Committee, International Congress on Industrial and Applied Mathematics (ICIAM) 2023.

E.4. Other notable professional activities

- AEOLUS team members organized multiple minisymposia at the 2021 SIAM Conference on Computational Science & Engineering; the 16th U.S. National Congress on Computational Mechanics; the 2021 SIAM Conference on Mathematical and Computational Issues in the Geosciences; the 2021 IFIP TC7 Conference on System Modelling and Optimization; 14th World Congress in Computational Mechanics; and the upcoming 2022 SIAM Conference on Uncertainty Quantification, among others.
- Biros is Member of the ACM/IEEE SC21 Test of Time Award Committee
- Biros serves as Program co-Chair, SIAM Parallel Processing for Scientific Computing 2020
- Biros serves on the ACM Gordon Bell Prize selection committee (6 members) 2018–
- Ghattas serves on the Editorial Board, Foundations of Data Science, 2019–
- Ghattas serves on the Advisory Board, Data Centric Engineering, 2019–
- Ghattas serves on the External Advisory Board of CLDERA (CLimate impact: Determining Etiology thRough pAthways), Grand Challenge LDRD, Sandia National Laboratories, 2021–2025
- Ghattas serves on the External Scientific Committee of the Energy and Environment French Excellence Initiative led by the University of Pau, National Institute for Agronomy (INRA), and Institute for Research in Computer Science and Automation (INRIA) (2017–)
- Ghattas serves on the Scientific Advisory Board (SAB) of PalMod (German Paleo Climate Modeling Initiative, Germany (2016–2022)
- Ghattas served as Chair, SIAM Activity Group on Uncertainty Quantification, 2019–2020

- Ghattas serves on the Scientific Advisory Board for the Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, 2020–2026.
- Marzouk serves on the Advisory Board, UK EPSRC Computational Statistical Inference for Engineering and Security (CoSInES) program
- Marzouk serves on the Advisory Board, UK EPSRC ICONIC (Inference, Computation and Numerics for Insights into Cities) program
- Marzouk served on the external advisory board of the Sandia National Laboratories SECURE Grand Challenge, 2019–2021.
- Marzouk serves on the editorial boards of the SIAM/ASA Journal on Uncertainty Quantification (2015–present), SIAM Journal on Scientific Computing (2017–present), Data-Centric Engineering (2019–present), Foundations of Data Science (2019–present), and International Journal for Uncertainty Quantification (2010–present).
- Marzouk serves on the organizing committee of the DOE Workshop on Data Reduction for Science (2020–present).
- Oden was elected to the 2020 Department of Aerospace Engineering and Engineering Mechanics (ASE/EM) Academy of Distinguished Alumni in the Cockrell School of Engineering at The University of Texas at Austin, Austin, Texas, April 17, 2020. The ASE/EM Academy of Distinguished Alumni was established to honor graduates of the aerospace, computational and engineering mechanics programs who have led distinguished careers in industry, government or academia, and to recognize their outstanding accomplishments.
- Webster serves as Editor-in-Chief, Numerical Methods for Partial Differential Equations; 2020 – present.
- Webster serves as Editor, Numerische Mathematik; 2019–present
- Webster serves as Editor, Results in Applied Mathematics; 2019–present
- Webster serves as President, SIAM Southeastern Atlantic Section; 2019–2021
- Willcox serves as Co-Chair of the NSF Advisory Committee for Cyberinfrastructure (ACCI), 2020–2022
- Willcox served as Chair of the AIAA Multidisciplinary Design Optimization Technical Committee, 2019–2021
- Willcox serves on the National Academies Board on Mathematical Sciences and Analytics (BMSA), 2016 – present
- Willcox serves on the Board of Trustees of the American Institute of Aeronautics and Astronautics (AIAA), 2020–2023
- Willcox serves on the Board of Advisors of the new Institute for Mathematical and Statistical Innovation, 2020–
- Willcox serves as inaugural Program Director, SIAM Activity Group on Data Science, 2020–2021