AEOLUS: Advances in Experimental Design, Optimal Control, and Learning for Uncertain Complex Systems
Center Progress Report: Year 2 (Sept 2019–Sept 2020)

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, all in the context of complex, uncertain energy systems. The AEOLUS center 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 second 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 17 highlights to feature here. The full spectrum of research is represented by the 44 publications that have appeared or been accepted during the reporting period (Appendix C.1) and the 23 others that have been submitted (Appendix C.2).

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. Bayesian inference, optimal experimental design, and optimal control with application to nanomanufacturing

In this section we describe research advances in forward modeling (§2.1), Bayesian inference (§2.2), optimal control (§2.3), and model inadequacy (§2.4) for block copolymer melts.

2.1. Analysis and fast algorithms for forward modeling of block copolymers systems

We continued to investigate mathematical and computational models for the microphase separation of block copolymer (BCP) melts. In particular, our effort has focused on two popular equilibrium continuum models: the Ohta-Kawasaki (OK) model, often referred to as the nonlocal Cahn-Hilliard model, and the self-consistent field theory (SCFT) model. The physical origins of the models were studied and efficient numerical algorithms for obtaining solutions were developed. We also developed a model that takes into account thermal annealing in the microphase separation process.

Mathematical analysis of the SCFT model derivation has been undertaken. This work involved analysis of essential steps in transforming the particle-based model of BCP phase change into the SCFT model. Major topics investigated included the statistical model of a single polymer chain, path integral formulation of the statistical field theory, and saddle-point approximation of the field-based Hamiltonian. This work also included a mathematically rigorous description of the particles-to-field transformation in statistical field theory with application to BCP, a topic absent from the existing literature.

We also continued to develop fast numerical algorithms and computer code for numerical solutions of the OK model. We proposed a fast and robust scheme for the direct minimization of the OK energy [9]. The scheme follows a globally convergent modified Newton method which is shown to be mass-conservative, energy-descending, and typically *three orders of magnitude faster* than the commonly-used gradient flow approach. The regularity and the first-order condition of minimizers were carefully analyzed. We conducted numerical studies of chemical substrate guided directed self-assembly of BCP melts, based on a novel polymer-substrate interaction model and the proposed scheme.

Besides the nonlocal Cahn-Hilliard and SCFT models described above, we also developed a model describing thermal annealing of BCPs, in which the mixture is rapidly quenched to a temperature below a critical temperature, leading to micro-phase separation. Simulating the thermal annealing process enables optimal control of the temperature change during self-assembly to achieve a defect-free BCP. We model this phenomenon by including thermal effects in the nonlocal Cahn-Hilliard model. The temperature significantly changes the polymer characteristics, including chain mobility and the Flory-Huggins parameter χ, and thus the nonlocal Cahn-Hilliard parameters ε and σ.

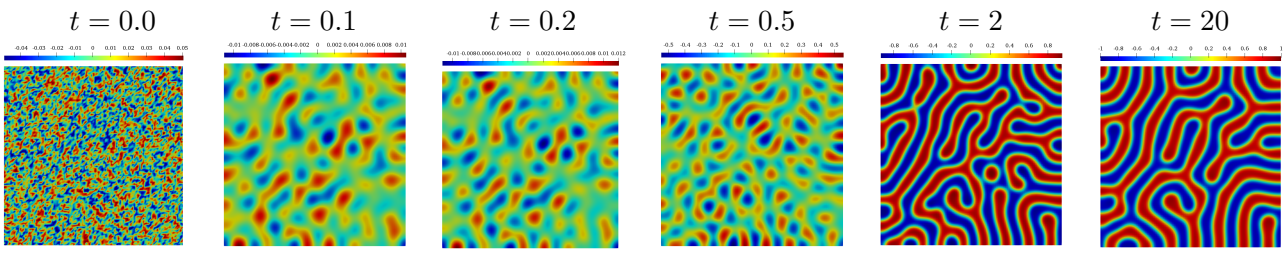


Figure 1: Simulating BCP thermal annealing using coupled nonlocal Cahn-Hilliard–thermal transport model. Starting with the polymer mix at $t = 0$, temperature is reduced below the critical temperature between $t = 0.1$ and $t = 0.2$.

Thermal transport in nano-scale polymer thin films is dominated by scattering of energy carriers at various surfaces or boundaries. The polymer chains are randomly coiled in bulk polymers, which shortens the mean free path of heat-carrying phonons. To address the competition between ballistic phonon transport and diffusive phonon transport in the polymer chain, we make use of a nonlocal heat conduction model. The resulting coupled nonlocal Cahn-Hilliard–thermal transport model is given by

$$\begin{aligned} \frac{\partial u}{\partial t} &= M_0 \exp(-\frac{\Delta E_a}{RT}) \left[\Delta(W' - \frac{\alpha T}{\chi_H + T\chi_S}\nabla u) - \frac{\beta T}{\chi_H + T\chi_S}(u - m) \right], \\ \frac{\partial T}{\partial t} &= k\nabla^2 T + k\tau_{en}\frac{\partial}{\partial t}(\nabla^2 T) + Q. \end{aligned}$$

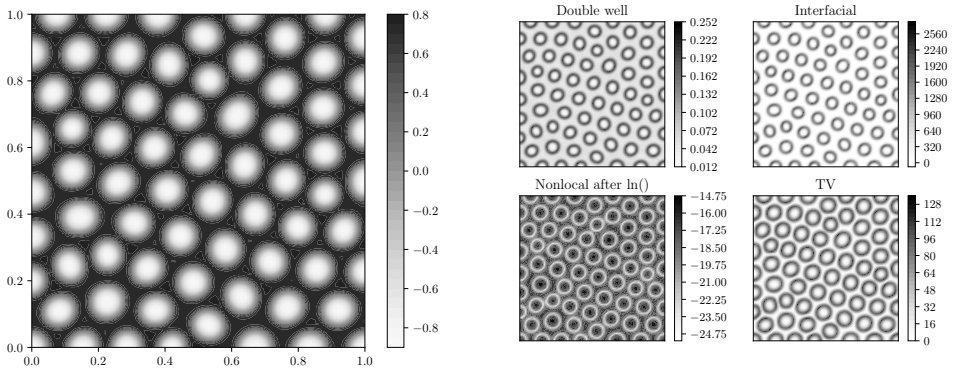
where u is the order parameter, M_0 is the temperature-independent mobility parameter, ΔE_a is the activation energy of the block copolymer, R is the ideal gas constant, T is temperature, W is the double well potential, α and β are material parameters, χ_S and χ_H are entropic and enthalpic Flory-Huggins parameters, m is the mass average of u, k is the thermal conductivity, the time scale τ_{en} acts as a retarding source to characterize the small spatial scale response, and Q is the (controllable) external heat source for annealing. Figure 1 shows numerical simulation results for the coupled system. The proposed coupled nonlocal Cahn-Hilliard–thermal transport model allows prediction of the comprehensive multiphysics phenomena involved in the BCP synthesis process, a topic absent from the existing literature. Additionally, the model enables optimizing the thermal annealing conditions during self-assembly to achieve desired nano-patterns useful in semiconductor applications.

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

2.2. Bayesian inference with uncertain models, with application to inference of nonlocal Cahn–Hilliard model parameters

We have investigated the Bayesian inference problem for phase separation of diblock copolymer (DBCP) melts with the Ohta-Kawasaki (OK) model. For given noisy images of the equilibrium morphology of DBCP melts, obtained either from experiments or from self-consistent field theory simulations, we seek to learn the corresponding OK model parameters via the framework of Bayesian inversion. In [5], we address two fundamental challenges: (1) identification of appropriate observational quantities of interest (QoIs); (2) the non-uniqueness of the OK model solution, a proxy for model uncertainty.

Identification of appropriate QoIs. The equilibrium morphologies of DBCP phase separation typically exhibit mesoscale ordered structures, such as lines, cylinders, and stacked balls. We proposed energy-based and Fourier-based QoIs that capture the essence of these structures from the given images, such as feature size, interfacial width, and feature periodicity. In addition, energy-based QoIs includes three OK-energy-inspired QoIs and a total-variation-inspired QoI. Visualization of the energy-based QoIs for a model solution is depicted in Figure 2, showing that the energy-based QoIs are representative of geometric features in the equilibrium states of DBCP phase separation. The Fourier-based QoIs are quantities that characterize the profile of the radial magnitude spectrum for the given noisy image, such



(a) A model solution

(b) The integrand of the energy-based QoIs for the model solution

Figure 2: The model solution and the integrand of the energy-based QoIs.

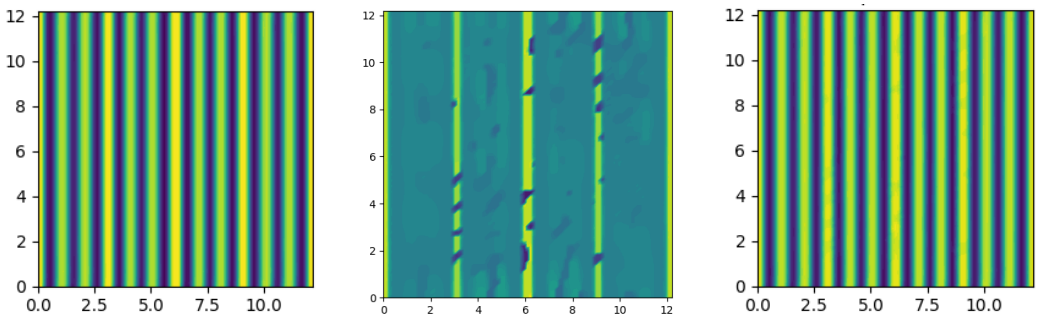
as the dominant radial frequency. Together these QoIs enable the interpretable and automatic characterization of DBCP equilibrium morphologies and their inherent structures, despite the large variance across images. Thus they serve as meaningful observable from which to inverse model parameters.

The non-uniqueness of the OK model solution. Due to the non-uniqueness of local minimizers of the OK energy, the solutions of the forward problem lead to a distribution of QoIs for a fixed set of model parameters. The distribution of QoIs can be seen as a form of model uncertainty that accounts for unknown influences (such as defects) on the formation of the equilibrium states that cannot be captured by the OK model. A commonly-adopted practice to characterize this uncertainty is to use isotropic random fields to access the local minimizers of the OK energy, thus leading to an intractable likelihood function. To address this challenge, we developed a likelihood-free approximate Bayesian computation method for the inference problem. We took the measure transport based variational density approximation approach, in which the joint density of model parameters, the QoIs, and the nuisance variable are characterized with parameterized transport maps. The transport approach relies on monotonic and triangular maps that enable the depiction of conditional distributions, such as the posterior, and whose invertibility allows sampling at low cost. The approach also enables one to compute the expected information gain (EIG) from the prior to the posterior, which gives us quantitative information about how much one can expect to learn from the data. Overall, our framework provides a systematic and computationally tractable approach for quantifying the utility of data in a Bayesian inverse problem that is otherwise intractable with traditional likelihood based methods.

Researchers: Ricardo Baptista (MIT), Lianghao Cao (UT), Joshua Chen (UT), Omar Ghattas (UT), Fengyi Li (MIT), Youssef Marzouk (MIT), and J. Tinsley Oden (UT)

2.3. Optimal control of nonlocal Cahn-Hilliard models, with application to directed self-assembly of block copolymers

We have addressed the problem of designing optimal chemical substrate patterns to direct phase separation of BCPs to form morphologies of interest. To model the phase separation process, we adopt the Ohta-Kawasaki model with an additional energy term representing the effects of the substrate chemical, and solve the resulting forward problem using the energy minimization framework of §2.1. We assume a thin polymer film and hence uniformity in the thickness, allowing us to approximate the phase field on a 2D domain. We formulate the optimal control problem in terms of a 2D control field representing the substrate chemical, leading to an infinite dimensional optimization problem. We seek controls whose values are binary, representing either a neutral or attractive chemical substrate. We desire sparse controls that take advantage of the natural density multiplication behavior of BCPs to ensure manufacturability of desired substrate patterns. Sparsity is enforced through the use of constraints and



(a) Target state **(b)** Optimal control **(c)** Optimal state

Figure 3: Example optimal control solution for a synthetically generated striped target morphology

sparsity-enhancing penalty functions in the control objective. The resulting optimization problem is solved by an infinite-dimensional Newton method, with derivatives obtained using the adjoint method.

Solutions of the optimal control problem demonstrate the ability to produce sparse controls that achieve the desired target morphologies (Figure 3) at a cost, measured in forward BCP model solves, that is independent of the control or state dimension. This work revealed several challenges that we are currently addressing, including the existence of multiple forward solutions and the enforcement of sufficient sparsity in the optimal control. Moreover, the next phase of this work will incorporate the effects of uncertainties stemming from Bayesian model calibration (§2.2) as well as model uncertainties (§2.4), capitalizing on our recent developments in stochastic optimization methods with infinite dimensional random parameter and optimal control fields [1, 10, 11, 20].

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

2.4. Representing model inadequacy, with application to nonlocal Cahn-Hilliard models of block copolymer model upscaled from self consistent field theory

Discrepancies between model outputs and observations from experiments or higher fidelity models are ubiquitous. When these discrepancies are larger than observational uncertainty, they can be attributed to some type of model inadequacy, which may arise due to many factors, including miscalibrated parameters or, more importantly, neglected or approximated physics. In making predictions, particularly of quantities that have not been experimentally observed—e.g., because the prediction scenario is not accessible in the lab or because the quantity of interest is not experimentally measurable—it is crucial to account for the effects of this model inadequacy. We are developing representations to quantify the effects of model inadequacy on predictions of diblock copolymer melts made using the nonlocal Cahn-Hilliard model.

In previous work, it has been found that when models of higher fidelity than the target model are available, they can provide important information for the construction and calibration of an inadequacy representation [19, 24]. Thus, as a starting point, the development of the nonlocal Cahn-Hilliard model as an approximation to self-consistent mean field theory (SCMFT) [12] has been analyzed. This analysis reveals three key approximations. First, the SCMFT is linearized about an infinite temperature state. Second, the domain of the melt is assumed large relative to the Kuhn statistical length. Third, the linear relationship between the mean density and the potential is approximately inverted, allowing the potential to be eliminated so that the governing equations can be written purely in terms of the density.

The first of these assumptions clearly introduces model inadequacy, but perturbing this assumption leads to analytical challenges. Thus, for now, this linearization is kept, although it will be examined further in future work. The second assumption is valid for the problems of interest and thus introduces no significant inadequacy. The third assumption introduces an inadequacy that is significant to the model predictions and can be perturbed in an analytically tractable fashion. Specifically, an approximate inverse

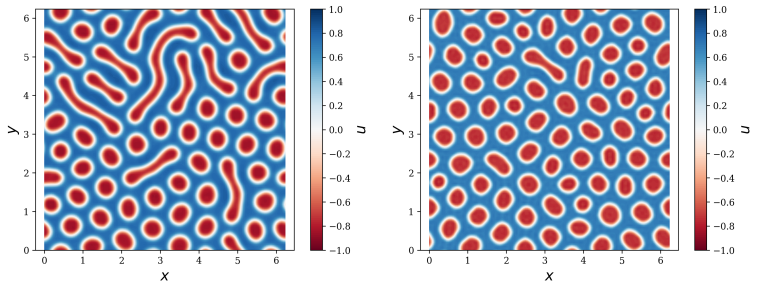


Figure 4: Original (left) and effect of perturbed long/short wave approximation blending (right) in nonlocal Cahn-Hilliard phase field model

is constructed by summing the inverses of long and short wave approximations of the true operator, but this blending is arbitrary. By replacing the blending we arrive at a family of models that can be used to quantify the impact of this modeling approximation. This family includes the original nonlocal Cahn-Hilliard model of course, which is nonlocal due to an inverse Laplacian in the free energy, as well as models that incorporate additional fractional Laplacian terms. These terms can have a substantial impact on the resulting solution of the phase field model, as shown in Figure 4.

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

3. Multiscale modeling and learning reduced order models, with application to additive manufacturing

In this section we describe research advances in multiscale (§3.1), reduced order (§3.2), and nonlocal interface (§3.3) modeling for solidification in additive manufacturing.

3.1. Multiscale modeling

We have implemented a two-dimensional multiscale model for investigating the effects of macroscopic heat transfer on the evolution of microstructure during additive manufacturing for binary alloys [3, 14]. The macroscopic model is a nonlinear heat equation that models the process of melting and solidification in the presence of a localized laser heat source. The microscopic model is a phase field (PF) model that describes the evolution of an order parameter and a concentration field to capture the complex microstructure pattern formation with anisotropic growth and noise-induced side-branching. We adopt a one-way macro-micro coupling approach (Figure 5) in which thermal gradient $G(t)$ and pulling velocity $R(t)$ are sampled along the trajectories tracking the solid-liquid interfaces from the macro-solver, and then supplied to the PF model as time-dependent parameters for microscopic simulations of directional solidification. Although this one-way coupling approach significantly reduces the computational cost of a fully coupled model, solving the PF equations is still computationally demanding due to the large spatial resolution required to resolve the thin, rapidly evolving interface on the micro-scale.

To address this challenge, we have implemented the PF model with a standard finite difference discretization and explicit time marching on graphics processing units (GPUs). The GPU-accelerated code uses *nonlinear preconditioning* to allow accuracy to be retained with fewer grid points along the interface than typically possible. The use of GPU acceleration and nonlinear preconditioning can substantially reduce the computational time of PF simulation for each $\{G(t), R(t)\}$ trajectory obtained from the macro-solver; this allows us to launch an ensemble of microscopic simulations to generate statistical information of quantities of interests (QoIs). We have also created a library of algorithmically generated QoIs to quantify microstructure material properties, including primary/secondary dendritic arm spacing, interfacial length, solid fraction, permeability and concentration variability [14]. Preliminary results suggest that the time-dependent thermal history has a strong influence on the field evolution and the QoIs of microstructure. We are currently developing a reduced order model that predicts the QoIs by interpolation techniques to limit the number of microscopic PF simulations.

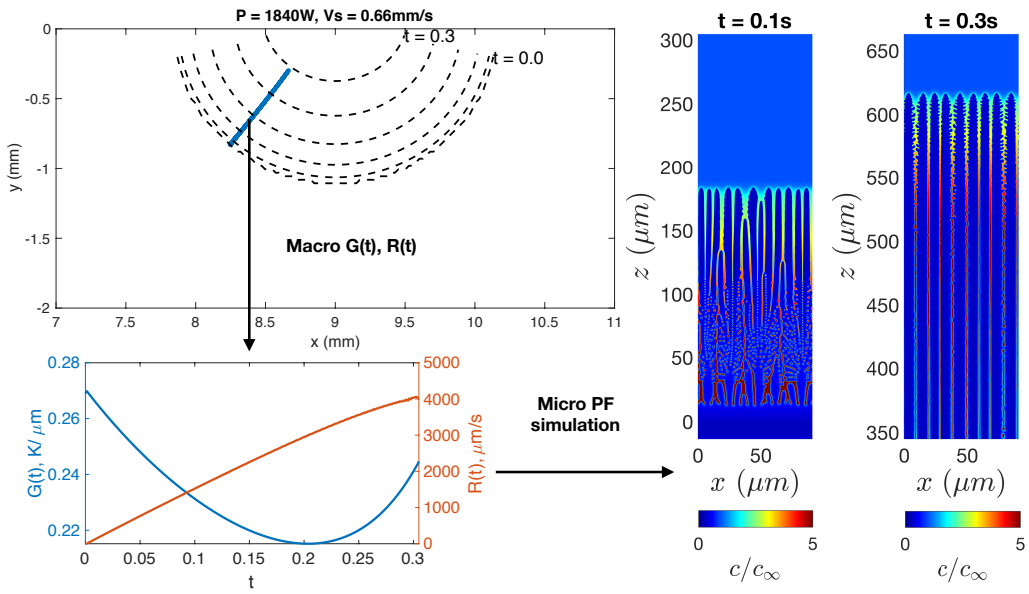


Figure 5: Illustration of macro-micro coupling, showing the level sets of the phase boundary in the macro-model (top left), the thermal gradient and solidification rate extracted from the macro-model (bottom left), and the time evolution of the micro-scale composition fields (right).

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

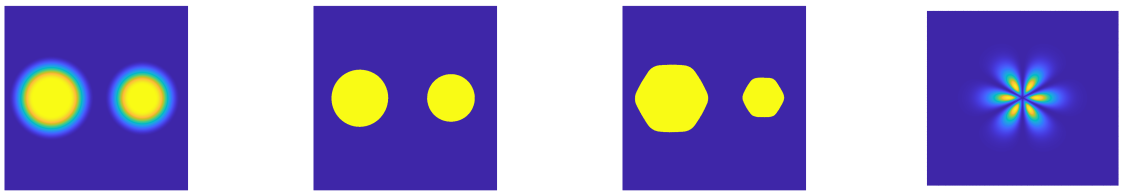
3.2. Operator inference for reduced-order modeling

We have continued to develop our Operator Inference approach, summarized in last year's report, for learning reduced-order models from simulation data. The non-intrusive nature of the Operator Inference approach enables variable transformations that expose system structure. This system structure defines the form of the reduced model, parameterized by reduced-order operators. We determine these operators by solving a linear least squares regression problem that minimizes the residual of the reduced model when applied to projected snapshot data. This year we have advanced the formulation robustness and algorithmic scalability of the approach. Regularization has been introduced to the formulation to avoid over-fitting. Over-fitting can arise due to the errors introduced by numerically estimating time derivatives, model mis-specification (i.e., the form of the system is not exactly as parameterized in our formulation), and/or truncated POD modes that leave some system dynamics unresolved. Over-fitting has been found to be a critical issue in our target additive manufacturing problems, particularly because the moving solidification front is difficult to approximate in a low-dimensional basis. We have shown that with appropriate regularization and an informed selection of learning variables, the Operator Inference reduced-order models exhibit high accuracy in re-predicting training conditions and acceptable accuracy in predictions for parameters not in the training data. We have released an open-source implementation of the Operator Inference method, together with tutorial examples [22].

Researchers: Stephen DeWitt (ORNL), Rudy Geelen (UT), Parisa Khodabakhshi (UT), Shane McQuarrie (UT), Balasubramaniam Radhakrishnan (ORNL), Karen Willcox (UT)

3.3. Nonlocal interface models for solidification

Phase field approaches are commonly applied for solidification modeling because they avoid having to explicitly track the interface, which instead is performed with a diffuse interface Cahn-Hilliard or Allen-Cahn model. Whereas these models are very versatile, they come with certain limitations. In particular, the thickness of the *diffuse* interface has to satisfy a model-dependent sharp- or thin-interface limit. For



(a) local **(b)** nonlocal **(c)** nonlocal anisotropic **(d)** anisotropic kernel

Figure 6: For the Cahn-Hilliard model, a comparison of local (a) and nonlocal (b) isotropic solutions and also an anisotropic nonlocal solution (c) corresponding to the nonlocal kernel (d).

common alloy solidification models, the thin-interface limit criterion is that the diffusion distance must be much larger than the interface width, which is a particular challenge under AM conditions. Violation of this condition leads to spurious solute-trapping effects and development of unphysical morphologies in the solidification microstructure. In order to satisfy the above condition, excessively fine meshes must often be employed in conventional model implementations, which leads to high computational cost.

To address this problem, we are developing new solidification models with nonlocal interface formulations, which permit *sharper* interfaces that can be simulated stably and accurately on coarser meshes. Here, we extend a recently developed framework for nonlocal Cahn-Hilliard models [8], where we have derived the necessary mathematical theory to show that, in contrast to the local model, the nonlocal solution can admit only pure phases (i.e., perfectly sharp interfaces) for non-vanishing nonlocal interactions (Figure 6a–b). We have also devised an efficient solution strategy that allows for the simulation of sharper interfaces independent of the grid spacing.

In our ongoing work, we are incorporating this model into solidification problems: we are developing nonlocal problem formulations based on the local Kobayashi and Wheeler-Boettinger-McFadden (WBM) models for pure materials and alloys, respectively. There, we replace the local operators for the phase field variable with nonlocal counterparts. Furthermore, to describe solidification problems that exhibit dendritic structure, anisotropy is introduced into the model. This is typically done by imposing highly nonlinear relations on the gradients of the phase field variable in existing local models. In contrast, the proposed nonlocal model is more versatile and allows for a wide variety of nonlocal interaction kernels (Figure 6d) and can realize complex anisotropy within a linear nonlocal operator (Figure 6c).

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

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, and uncertainty quantification 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. Second-order methods for stochastic optimization

We have developed efficient matrix free 2nd order methods for the solution of stochastic nonconvex optimization problems. We have specifically targeted empirical risk minimization, which arises in such settings as neural network training. The problem can be stated as $\min_w F(w)$ where F is a finite sum approximation of how well an approximant (neural network) can represent an input–output mapping $x \mapsto y$ over a joint probability $\nu(x, y)$. Stochastic nonconvex optimization problems are solved iteratively performing the weight update $w_{k+1} = w_k + \alpha_k p_k$, where w_k is the optimization variable at iteration k, p_k is a search direction, and α_k is the step length. Stochastic nonconvex optimization problems

are difficult for a number of reasons: the high dimensionality d_W of the optimization variables, the large cardinality N of the training data, the nonconvexity and ill-conditioning of the problem, and the stochasticity inherent in subsampling schemes used to reduce computational cost.

In the typical setting of large d_W and N, 2nd methods are seen as prohibitive, since there is a common misconception that the Hessian must be explicitly constructed. Instead, subsampled 1st order methods (e.g., stochastic gradient descent and its variants) are favored in practice. We have developed efficient 2nd order methods that outperform 1st order methods by approximating the Newton direction $p_k = -(\nabla^2 F(w_k))^{-1} \nabla F(w_k)$ via subsampling and matrix-free solvers [20]. Decays of typical empirical risk Hessian spectra show that matrix-free methods can approximate the dominant modes of the Hessian with a small number of Hessian-vector products using low rank decompositions and Krylov methods. Without having to densely form and factor the Hessian for inversion, these matrix-free Newton methods are comparable in per-iteration cost to subsampled 1st order methods, and require many fewer iterations.

Due to nonconvexity, gradient based optimizers may slow down in the vicinity of saddle points and indefinite regions. We exploit knowledge of the dominant modes of the Hessian spectrum—as revealed by randomized low rank eigenvalue decompositions—to facilitate fast escape from indefinite regions, leading to the *low rank Saddle Free Newton algorithm* (LRSFN) [21]. Due to ill-conditioning of the problem, 1st order methods are slow to converge. We show theoretically and experimentally that both low rank and Krylov methods for approximating the Newton direction can achieve faster asymptotic convergence than 1st order methods. Due to stochasticity, information in the training data can change drastically from one iteration to the next. We show both theoretically and experimentally that the information content of the dominant eigenvalues of the Hessian exhibit low variance with respect to subsampling. This has two practical benefits: (1) we can use fewer samples when approximating these modes, and (2) we can explicitly truncate modes that exhibit high variance and lead to overfitting.

In summary, our matrix-free Newton methods for stochastic optimization are comparable in per-iteration cost to 1st order methods and require many fewer iterations, improve convergence in the vicinity of local minima, facilitate fast escape from saddle points, and avoid overfitting by truncating high variance "noisy" modes of the empirical risk Hessian, leading to superior generalization properties.

Researchers: Nick Alger (UT), Omar Ghattas (UT), Tom O'Leary-Roseberry.

4.2. An adaptive stochastic gradient-free approach for high-dimensional optimization

As a complement to the Newton methods described in §4.1, recently we developed a novel adaptive stochastic gradient-free (ASGF) approach for solving high-dimensional nonconvex optimization problems based on function evaluations only [13]. We employ a directional Gaussian smoothing of the target function that generates a surrogate of the gradient and assists in avoiding "bad" local optima by utilizing nonlocal information of the loss landscape. Applying a deterministic quadrature scheme results in a massively scalable technique that is sample-efficient and achieves spectral accuracy. At each step we randomly generate the search directions while primarily following the surrogate of the smoothed gradient. This enables exploitation of the gradient direction while maintaining sufficient space exploration, and accelerates convergence towards global extrema. In addition, we make use of a local approximation of the Lipschitz constant in order to adaptively adjust the values of all hyper-parameters, thus removing the careful fine-tuning of current algorithms that is often necessary to be successful for a large class of learning tasks (e.g., training deep neural networks, maximizing rewards in reinforcement learning). As such, the ASGF strategy offers significant improvements when solving high-dimensional nonconvex optimization problems relative to other gradient-free methods (including "evolutionary strategies") as well as iterative approaches that rely on gradient information of the objective function.

We illustrate the improved performance of ASGF in the setting of high-dimensional optimization on 100, 1000, and $10,000$-dimensional benchmarks (Ackley, Levy, Rastrigin, and Sphere functions). All simulations converged successfully regardless of initial guess; specific optimization trajectories are

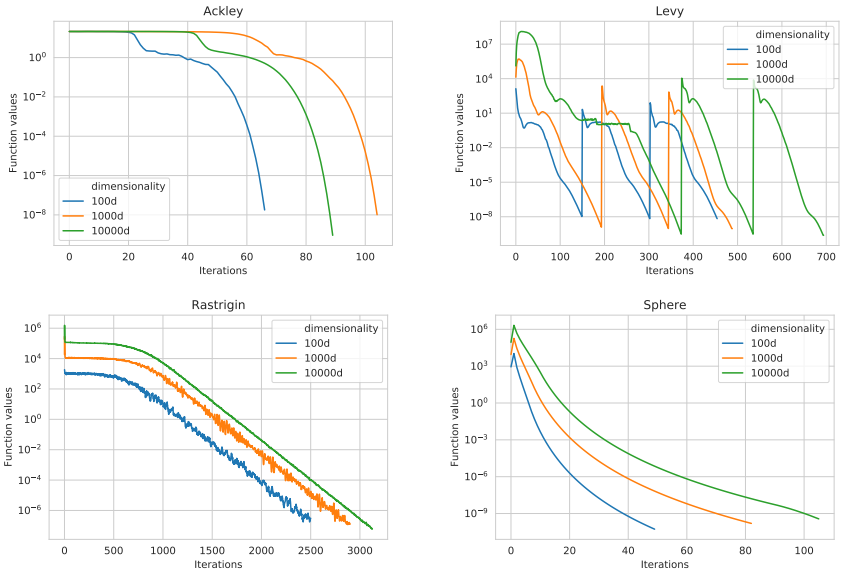


Figure 7: Performance of ASGF on high-dimensional test functions.

displayed in Figure 7. The average numbers of iterations and function evaluations are given in Table 1. We note that the irregularity of the optimization trajectories in Figure 7 for the Rastrigin function is caused by the highly oscillatory nature of the loss landscape. The irregularity on the Levy benchmark is due to the adaptive "parameter reset" feature of ASGF. In particular, it can be observed that the parameter reset indeed helps the algorithm to escape local optima and converge to the global minimum. In the cases of Ackley and Sphere functions, due to the distinct geometry of the global minimum, the parameter reset is not triggered, and hence the optimization trajectories are smooth.

Table 1: Average number of iterations and function evaluations of ASGF.

Benchmark	Iterations	Evaluations	Benchmark	Iterations	Evaluations
Ackley 100d	66	27,343	Rastrigin 100d	2,995	1,290,215
Ackley 1000d	103	414,298	Rastrigin 1000d	2,901	11,625,963
Ackley 10000d	89	3,548,775	Rastrigin 10000d	3,206	114,845,172
Levy 100d	452	184,176	Sphere 100d	48	19,381
Levy 1000d	508	2,037,076	Sphere 1000d	76	303,508
Levy 10000d	617	24,698,140	Sphere 10000d	112	4,480,337

Researchers: Anton Dereventsov (ORNL), Max Gunzburger (UT), Clayton Webster (UTK)

4.3. Approximation and estimation of transport maps

The construction of transport maps that deterministically couple a simple/tractable "reference" probability distribution with a more complex "target" distribution of interest is useful for a host of AEOLUS problems. Specifically, these maps underpin:

- *Variational approaches to Bayesian inference,* e.g., minimization of the Kullback–Leibler divergence $D_{\mathrm{KL}}(T_\sharp\rho\|\pi)$, where π represents the posterior distribution of interest, by providing rich and infinitely refinable classes of approximations induced by maps T. (Here $T_\sharp\rho$ denotes the pushforward of the reference ρ under T.) Stein variational methods, which have been advanced under AEOLUS and described in previous reports, construct nonparametric approximations of T within this framework.
- *Density estimation and generative modeling:* Given samples from a target distribution π, we may need to estimate the probability density function of π and generate additional samples. This applies directly to estimation of information gain objectives in optimal Bayesian experimental design (see §4.4, §2.2).

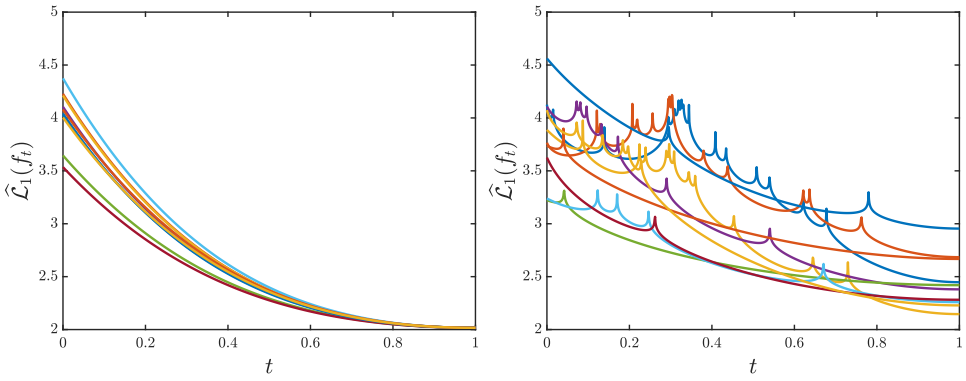


Figure 8: Objective functions for map estimation from samples, using either the new representation described in §4.3 or an earlier sum-of-squares monotone parameterization. The objective is evaluated along line segments that interpolate between random initial maps ($t = 0$) and critical points resulting from a gradient-based optimization method ($t = 1$). With the new representation (*left*) the algorithm always arrives at the same optimal value (at $t = 1$), whereas with the previous approaches (*right*) the algorithm gets stuck in local minima and rarely attains the optimal value.

- *Likelihood-free inference:* In many inference problems, we may be able to only simulate (i.e., draw samples from) the conditional distribution of the data $\pi(y|x)$, and even the prior $\pi(x)$, yet we still wish to characterize the posterior distribution of the parameters $\pi(x|y)$. Here, standard Bayesian tools that require unnormalized evaluations of the posterior density, like MCMC or variational inference, do not directly apply. A demonstration of likelihood-free inference for parameters of the nonlocal Cahn-Hilliard model is described in §2.2.

Succesfully solving problems in any of these three classes requires the ability to parameterize and learn transport maps with controlled accuracy and computational effort. This need has motivated fundamental work aimed at understanding the *approximation* of transport maps, the construction of new map parameterizations, and the development of new statistical *estimators* that achieve good performance in the small-sample regime. We review our recent efforts below.

In [26], we developed a first analysis of the approximation of triangular transport maps, by polynomials or neural networks, on bounded domains. Our results extend to the case of infinite-dimensional parameters, given suitable reference and target measures. Specifically, let ρ and π be two probability measures on $[-1,1]^d$ with positive and analytic Lebesgue densities. We investigate the approximation of the unique triangular monotone (Knothe–Rosenblatt) transport $T : [-1,1]^d \to [-1,1]^d$, such that the pushforward $T_\sharp\rho$ equals π. We show that for $d \in \mathbb{N}$ there exist approximations $\tilde{T}$ of T based on either sparse polynomial expansions or ReLU networks, such that the distance between $\tilde{T}_\sharp\rho$ and π decreases exponentially. More precisely, we show error bounds of the type $\exp(-\beta N^{1/d})$ (or $\exp(-\beta N^{1/(d+1)})$ for neural networks), where N refers to the dimension of the ansatz space (or the size of the network) containing $\tilde{T}$; the notion of distance comprises, among others, the Hellinger distance and the Kullback–Leibler divergence. The construction guarantees $\tilde{T}$ to be a monotone triangular bijective transport on the hypercube $[-1,1]^d$. Analogous results hold for the inverse transport $S = T^{-1}$. The proofs are constructive, and we give an explicit *a priori* description of the ansatz space, which can be used for numerical implementations. Additionally we discuss the high-dimensional case: for $d = \infty$ a dimension-independent algebraic convergence rate is proved for a class of probability measures occurring widely in Bayesian inference for inverse problems, thus verifying that the curse of dimensionality can be overcome in this setting.

Turning now to the *statistical* problem of estimating transport maps from samples, we have developed new parameterizations and adaptive algorithms for building triangular maps on unbounded domains. Triangular maps define an autoregressive model where each component represents one marginal conditional in the factorization of π. Despite the empirical success of different map parameterizations [17, 18], little

work has addressed the properties of the *optimization problems* involved in estimating triangular transport maps. In [4], we have developed a systematic framework for representing and learning monotone triangular maps. Our approach relies on an operator that transforms broad classes of smooth functions into monotone functions. From the theoretical perspective, we show that the associated optimization problem is *well-defined* and *continuous* under appropriate tail conditions; we also demonstrate that it has a unique global minimum (see Figure 8). Algorithmically, we then describe an adaptive procedure for selecting appropriate smooth functions given a hierarchical basis of the corresponding function space. The procedure naturally produces map representations that are parsimonious and interpretable—in the sense that it exploits and implicitly discovers conditional independence. Maintaining a strict triangular structure also exposes certain block conditionals, immediately enabling *conditional density estimation* and likelihood-free inference. Our numerical experiments show that the algorithm provides robust performance at small-to-moderate sample sizes, and constitutes a semi-parametric approach that naturally links map complexity to the size of the data.

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

4.4. Optimal experimental design

We have developed a fast and scalable computational framework to solve large-scale and high-dimensional Bayesian optimal experimental design problems. In particular, we consider the problem of optimal observation sensor placement for Bayesian inference of high-dimensional parameters governed by partial differential equations (PDEs), which is formulated as an optimization problem that seeks to maximize an expected information gain (EIG). Such optimization problems are particularly challenging due to the curse of dimensionality for high-dimensional parameters and the expensive solution of large-scale PDEs. To address these challenges, we exploit two essential properties of such problems: (1) the low-rank structure of the Jacobian of the parameter-to-observable map to extract the intrinsically low-dimensional data-informed subspace, and (2) the high correlation of the approximate EIGs by a series of approximations to reduce the number of PDE solves. Based on these properties, we propose an efficient offline–online decomposition for the optimization problem: an offline stage in which a limited number (independent of the parameter and data dimensions) of forward/adjoint PDEs are solved, and an online stage of optimizing sensor placement, which does not require any PDE solves. For the online optimization, we propose a swapping greedy algorithm that first constructs an initial set of sensors using leverage scores, and then swaps the chosen sensors with other candidates until certain convergence criteria are met. We demonstrate the efficiency and scalability of the proposed computational framework via a linear inverse problem of inferring the initial condition for an advection-diffusion equation, and a nonlinear inverse problem of inferring the diffusion coefficient of a log-normal diffusion equation, with both the parameter and data dimensions ranging from a few tens to a few thousands. Figure 9 shows the approximate EIG by the swapping greedy and the standard greedy algorithms, compared to the EIG for all possible designs for 9 candidate sensors and 200 random designs for 81 candidate sensors. The results demonstrate near optimality at a cost of few PDE solves in a dimension-independent algorithm.

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

4.5. Robust linear filtering and experimental design for systems governed by stochastic differential equations (SDEs) under model uncertainty

It is common practice in signal processing to begin with a stochastic-process model (signal plus noise), a covariance (or power spectra) model, or a state-observation model, as with Kalman filtering. However, in a physical context, the signal model may be derived from a physical model, which can be a parameterized mathematical system. Hence, the properties of the signal, and of the resulting filter, depend on the physical model, and the signal parameters are expressed in terms of the parameters of the physical model.

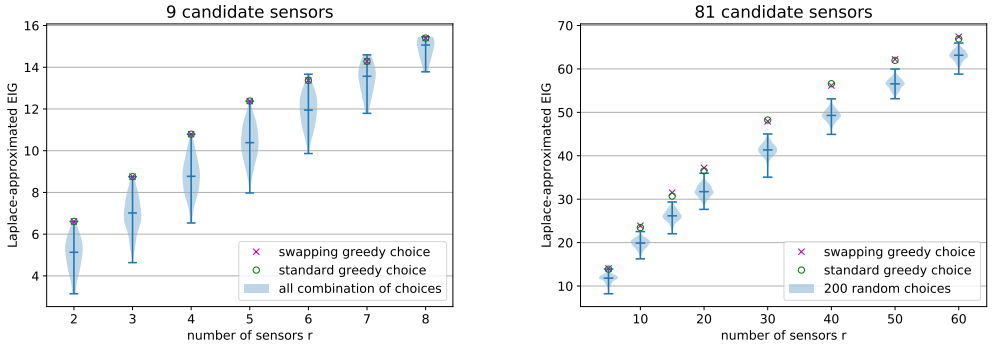


Figure 9: Laplace approximate EIG with increasing number of sensors out of 9 (left) and 81 (right) candidates. Blue filled area represents the probability of $\hat{\Psi}$ for all the designs with lines at the minimum, maximum and median.

If there is uncertainty with regard to some parameters in the physical model, this uncertainty is then propagated to the signal model, for instance, uncertainty in the covariance matrix. The key factor for our work is that, if the uncertainty in the physical model arises from lack of scientific knowledge and the uncertainty is characterized by a prior distribution governing the uncertain (random) parameters, thereby characterizing our scientific understanding of the uncertainty, then that prior distribution continues to govern the uncertain parameters in the signal model. In summary, both the signal model and its uncertainty are dictated by the physical model, and not hypothesized independently.

In [27] we derived robust linear filtering and experimental design for systems governed by stochastic differential equations (SDEs) under model uncertainty. Given a model of signal and observation processes, an optimal linear filter is found by solving the Wiener-Hopf equation; with model uncertainty, it is desirable to derive a corresponding robust filter. Our work assumes that the physical process is modeled via an SDE system with unknown parameters; the signals are degraded by blurring and additive noise. Due to time-dependent stochasticity in SDE systems, the system is nonstationary, and the resulting Wiener-Hopf equation is difficult to solve in closed form. Hence, we discretized the problem to obtain a matrix system to carry out the overall procedure. We further derived an intrinsically Bayesian robust (IBR) linear filter together with an optimal experimental design framework to determine the importance of the SDE parameter(s). We applied the theory to SDE-based model dynamics. Furthermore, we applied our robust operator and experimental design framework to uncertain systems described by coupled ordinary differential equations (ODEs) [16], where we demonstrated the clear advantages of our objective-based uncertainty quantification (objective-UQ) approaches. Our recent work extends the objective-UQ framework to encompass multi-objective optimization under model uncertainty [25].

Researchers: Francis J Alexander (BNL), Edward Dougherty (TAMU), Omar Maddouri (TAMU), Xiaoning Qian (TAMU), Byung-Jun Yoon (TAMU), Guang Zhao (TAMU)

4.6. Multifidelity methods for nonlocal problems

Nonlocal models (§3.3 and §4.8) are generally more expensive computationally compared to their local counterparts due to reduced sparsity. Hence, a multifidelity method [23] that combines surrogate models of lower fidelity with the high-fidelity model can be useful for reducing the computational costs of nonlocal models. We examine this conjecture using the one-dimensional nonlocal diffusion problem

$$-2\int_{-\delta}^{L_0+\delta} (u(y)-u(x))\,\gamma dy = z_1 \;\; \forall x \in (0, L_0), \quad u = z_2 \;\; \forall x \in [-\delta, 0], \quad u = 0 \;\; \forall x \in [L_0, L_0+\delta],$$

where L_0 is the length of the domain, δ is the nonlocal horizon, and the source term z_1 and volume-constrained data z_2 are independent and uniformly distributed random variables in $[0.9, 1.1]$. The truth or target value for the QoI $\mathbb{E}[u(0.5)]$ is calculated as the Monte Carlo (MC) estimate with $N = 10^5$

	Model	h	δ	w_i/w_1	$\rho_{1,i}$
$f^{(1)}$	High fidelity: fine grid, largest horizon	$1/2^{10}$	0.25	1.000	1.000000
$f^{(2)}$	Coarse grid, largest horizon	$1/2^{9}$	0.25	0.145	0.999994
$f^{(3)}$	Coarsest grid, largest horizon	$1/2^{8}$	0.25	0.024	0.999948
$f^{(4)}$	Coarsest grid, 20% reduction in the horizon	$1/2^{8}$	0.20	0.018	0.999366
$f^{(5)}$	Coarsest grid, 40% reduction in the horizon	$1/2^{8}$	0.15	0.012	0.998263

Table 2: Multifidelity models for nonlocal diffusion problem, together with their costs and QoI correlation coefficients estimated from 500 samples.

samples of the high-fidelity model with $\delta = 0.25$ and $h = L_0/2^{10}$. We consider the five models listed in Table 2, which include the high-fidelity truth model and four models of lower fidelity. Our approach uses multifidelity Monte Carlo (MFMC) to optimally allocate the number of evaluations among each model, based on the computational costs w_i and the correlations $\rho_{1,i}$ with the high-fidelity model. The estimated mean-squared error (MSE) for different choices of MFMC estimators and the distribution of the total number of samples between different models is shown in Figure 10. To our knowledge, this is the first application of multifidelity methods to accelerate computations for nonlocal problems.

Researchers: Max Gunzburger (FSU/UT), Parisa Khodabakhshi (UT), Karen Willcox (UT)

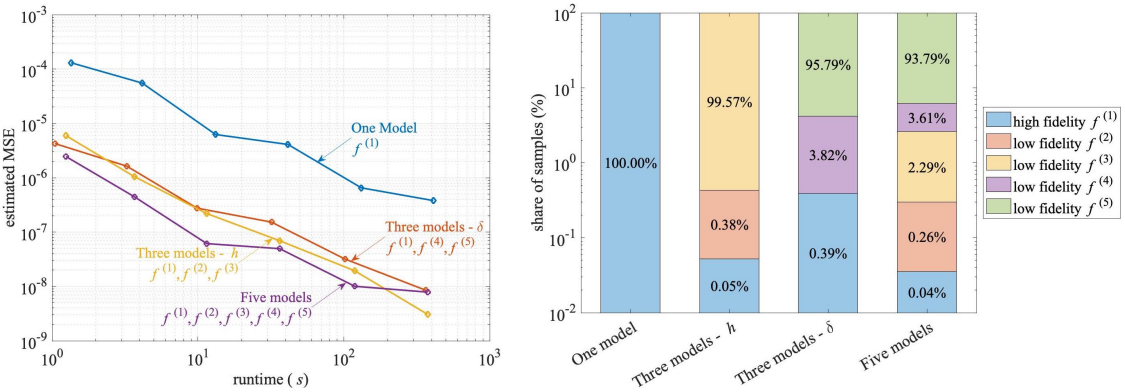


Figure 10: Left: For the same MSE, speedups of up to three orders of magnitude are achieved using the MFMC approach. Right: Very few samples are taken of the high-fidelity model with the majority of samples taken for the least costly models.

4.7. Reduced order models with memory effects

Model reduction of dynamical systems with unresolved degrees of freedom (DOFs) leads to memory effects in the form of a kernel integral operator acting on the time history of the resolved DOFs. In this work, we employ a data-driven approach to study the inverse problem of reconstructing the memory kernel operators for linear dynamical systems [2]. The inverse problem is classified into two types depending on the availability of data: (1) full observation when data for both resolved and unresolved DOFs are available for reconstruction, and (2) partial observation when only data for resolved DOFs are available. Our main theoretical contribution is that the inverse problem of type 1 is well-posed for both constant- and variable-coefficient linear dynamical systems, and the type-2 problem is ill-posed for variable-coefficient systems. For each problem type we propose solution methodologies for different variants of the inverse problem: full vs. truncated memory approximation, constant- vs. variable-coefficient systems, and dynamical systems with parametric dependence.

In the case of full-memory reconstruction, we develop fast solvers that exploit the block-triangular structure of the discrete inverse problem so that a large optimization problem can be decoupled into a number of small ones to be solved sequentially. To overcome the inherent ill-posedness of the inverse problem with partial observation, we use a Tykhonov-type regularization technique to enforce the continuity of the reconstructed operator in time. In the case of truncated memory reconstruction, however,

such a triangular solver is not possible and we have to solve a coupled optimization problem with a smaller size in the time dimension. The truncated memory kernel approximation performs particularly well for dynamical systems with (weakly) decaying kernels in time. Even for some oscillatory kernels, retaining 40% of the memory gives a reasonable prediction of the dynamics.

Researchers: Yuanxun Bao (UT) and George Biros (UT)

4.8. Nonlocal models

During the 1st project year an opportunity arose for introducing a nonlocal Cahn-Hilliard phase-field model relevant to co-polymer flows. The nonlocal models we use replace classical elliptic PDE operators by integral operators having the form $\int_{|\mathbf{y}-\mathbf{x}|\leq\delta}\gamma(\mathbf{x},\mathbf{y})\big(u(\mathbf{y})-u(\mathbf{x})\big)d\mathbf{y}$ for a given length scale δ and a given interaction kernel γ. Thus, points separated by a finite distance interact with each other. Nonlocal models have proven to be successful in a wide and diverse variety of settings including, among many others, fracture in solids, subsurface flows, and image processing. Furthermore, models of this type have, as special cases, many well known models such as spatially fractional diffusion and the peridynamics model for mechanics. The nonlocal interface model, when compared to classical ones, offer much greater flexibility; for example, they can produce sharp interfaces without the need for grid refinement near physical interfaces [8]. During the 2nd project year, several new opportunities for nonlocal modeling arose that have the potential of being more faithful to physics compared to PDE models. For example, in §3.3, we report on our preliminary work on nonlocal models for solidification relevant to additive manufacturing. Another nascent opportunity is the use of nonlocal Helmholtz equations for the design of cloaking materials that prevent the reflection of waves.

Nonlocality comes at a price: compared to PDEs, nonlocal discrete systems are less sparse, often much more so, so that both assembly and solution costs are greater. To address this issue and thus render nonlocal modeling truly useful in practice, we have initiated projects for reducing those costs in settings such as UQ and optimization that require multiple model solutions. In particular, for fractional-type nonlocal kernels we have developed an efficient reduced order model (ROM) strategy based on an affine-approximation of the nonlocal operator [7] and have successfully used it for optimization based parameter identification [6]. Furthermore, we are designing nonlocal multifidelity methods that leverage less expensive computational models (having smaller interaction length scales δ and larger grid sizes) to much more cheaply determine desired quantities at a chosen (largest) length scale and (smallest) grid size. We are also designing POD-based ROMs for the same purpose. Preliminary results for these efforts are reported in §4.6. We emphasize that the need for such approaches is much more acute and potentially much more effective in the nonlocal setting compared to the local PDE setting.

Researchers: Olena Burkovska (ORNL), Peng Chen (UT), Stephen DeWitt (ORNL), Max Gunzburger (UT), Parisa Khodabakhshi (UT), J. Tinsley Oden (UT), Balasubramaniam Radhakrishnan (ORNL), Clayton Webster (UTK), and Karen Willcox (UT)

4.9. Active learning

In supervised learning, labeling data is often expensive and highly time consuming. Active learning addresses this problem and has been demonstrated for sample efficient learning with less required labeled data. For pool-based active learning, in each 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 classification error given a new labeled candidate based on a one-step-look-ahead strategy. ELR is the optimal strategy with a single query; however, since such myopic strategies cannot identify the long-term effect of a query on the classification error, ELR may get stuck before reaching the optimal classifier. 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.

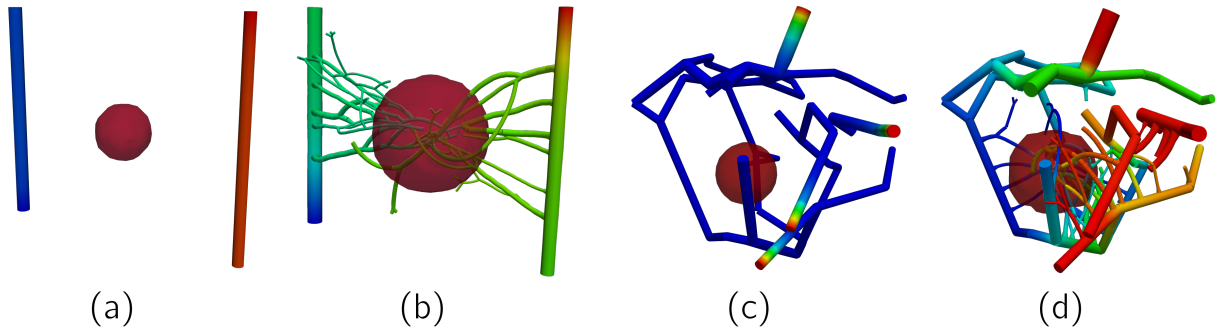


Figure 11: Angiogenesis effect. (a)–(b) initial and final view (two-vessels setting). (c)–(d) initial and final view (complex-network setting).

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 focus on the uncertainty directly related to classification error. In our work [29], we proposed active learning based on a weighted form of MOCU and proved that our proposed active learning algorithm converges to the optimal classifier of the true model. We further demonstrated its performance with both synthetic and real-world datasets. In our recent work [28], we proposed a strictly concave approximation of MOCU—referred to as *Soft MOCU*—that can be used to define an acquisition function to guide Bayesian active learning with theoretical convergence guarantees. For training Bayesian classifiers with both synthetic and real-world data, our experiments again demonstrated the superior performance of active learning by Soft MOCU compared to other existing methods.

Researchers: Francis J Alexander (BNL), Anthony DeGennaro (BNL), Edward Dougherty (TAMU), Omar Maddouri (TAMU), Xiaoning Qian (TAMU), Byung-Jun Yoon (TAMU), Guang Zhao (TAMU)

4.10. Nonlinear Phase Field Models of Vascular Tumor Growth

Generalization of the Cahn-Hilliard-type phase field model employed in simulating phase separation in block copolymers can be derived for a class of models of the growth of tumors in an evolving vascular network. In these models, the Ginsburg-Landeau energy functional involves terms similar to those in BCP except that multiple species of cell types and other constituents occur, with phase separation representing the transition of tumor cells from hypoxic to proliferative to necrotic depending on the local concentrations of nutrients. Other species, such as extracellular matrix, matrix-degenerative enzymes, and tumor-angiogenesis protein concentrations make up a system of multiple unknowns governed by a coupled system of nonlinear evolution partial differential equations, generally 10 unknown fields, with convective velocities of species governed by Darcy-type laws.

We are particularly interested in developing realistic models of angiogenesis, the phenomenon in which hypoxic tumor cells release tumor-angiogenesis factors (TAFs) that diffuse outside the tumor boundary and, upon contact with blood vessels at a sufficiently high concentration, promote growth of the vascular network so as to supply nutrients to the tumor and promote its continued growth (Figure 11). We have developed a unique class of 1D network models describing the vascular system that are embedded in the 3D model of the tumor mass. Of particular interest, we have developed a rigorous mathematical analysis of the well-posedness of the full 1D–3D model as well as parallel code implementing finite element discretizations of the full system [15]. We expect to secure data for model calibration and validation through a new project in collaboration with M.D. Anderson Cancer Center.

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)

References

[1] Ilona Ambartsumyan and Omar Ghattas. Fast and scalable methods for Bayesian inverse problems with uncertain PDE forward models. *In preparation*, 2020.

[2] Yuanxun Bao and George Biros. Reconstruction of memory kernel operators for linear dynamical systems. *In preparation*, 2020.

[3] Yuanxun Bao, George Biros, Stephen DeWitt, Yigong Qin, and Balasubramaniam Radhakrishnan. Validation of a multiscale phase-field model for binary alloy solidification in a weld pool. *In preparation*, 2020.

[4] R. Baptista, O. Zahm, and Y. M. Marzouk. An adaptive transport framework for joint and conditional density estimation. *arXiv:2009.10303, submitted*, 2020.

[5] Ricardo Baptista, Lianghao Cao, Joshua Chen, Omar Ghattas, Fengyi Li, Youssef Marzouk, and J. Tinsley Oden. Likelihood-free inference and information gain from images ofdiblock copolymer phase separation via measure transport. *https://www.dropbox.com/s/k8dp93r1o71dxou/main.pdf*, 2020.

[6] Olena Burkovska, Christian Glusa, and Marta D'Elia. An optimization-based approach to parameter learning for fractional type nonlocal models. *Submitted*, 2020. arXiv:2010.03666.

[7] Olena Burkovska and Max Gunzburger. Affine Approximation of Parametrized Kernels and Model Order Reduction for Nonlocal and Fractional Laplace Models. *SIAM Journal on Numerical Analysis*, 58(3):1469–1494, 2020.

[8] Olena Burkovska and Max Gunzburger. On a nonlocal Cahn–Hilliard model permitting sharp interfaces. *Submitted*, 2020. arXiv:2004.14379.

[9] Lianghao Cao, Omar Ghattas, and J. Tinsley Oden. Globally convergent direct minimization of the Ohta-Kawasaki energy with application to the directed self-assembly of diblock copolymers. *Draft*, 2020.

[10] Peng Chen, Michael Haberman, and Omar Ghattas. Optimal design of acoustic metamaterial cloaks under uncertainty. *Submitted*, 2020. https://arxiv.org/abs/2007.13252.

[11] Peng Chen, Umberto Villa, and Omar Ghattas. Taylor approximation and variance reduction for PDE-constrained optimal control under uncertainty. *Journal of Computational Physics*, 385:163–186, 2019. https://arxiv.org/abs/1804.04301.

[12] Rustum Choksi and Xiaofeng Ren. On the derivation of a density functional theory for microphase separation of diblock copolymers. *Journal of Statistical Physics*, 113(1-2):151–176, 2003.

[13] A. Dereventsov, C. G. Webster, and J. Daws. An adaptive stochastic gradient-free approach for high-dimensional blackbox optimization. In *Advances in Neural Information Processing Systems 32*. Curran Associates, Inc., 2020. Submitted (arXiv:2006.10887).

[14] Stephen DeWitt, Balasubramaniam Radhakrishnan, Yuanxun Bao, Yigong Qin, George Biros, and John Turner. Additive manufacturing testbed problems for mathematical method development. Technical report, Oak Ridge TN, 2020.

[15] 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. *arXiv preprint arXiv:2006.10477*, 2020.

[16] Youngjoon Hong, Bongsuk Kwon, and Byung-Jun Yoon. Optimal experimental design for uncertain systems based on coupled differential equations, 2020.

[17] Priyank Jaini, Kira A Selby, and Yaoliang Yu. Sum-of-Squares Polynomial Flow. In *International Conference on Machine Learning*, pages 3009–3018, 2019.

[18] Youssef Marzouk, Tarek Moselhy, Matthew Parno, and Alessio Spantini. *Sampling via Measure Transport: An Introduction*, pages 1–41. Springer International Publishing, 2016.

[19] Rebecca E Morrison, Todd A Oliver, and Robert D Moser. Representing model inadequacy: A stochastic operator approach. *SIAM/ASA Journal on Uncertainty Quantification*, 6(2):457–496, 2018.

[20] T. O'Leary-Roseberry, N. Alger, and O. Ghattas. Inexact Newton methods for stochastic non-convex optimization with applications to neural network training. *submitted*, 2019. https://arxiv.org/abs/1905.06738.

[21] T. O'Leary-Roseberry, N. Alger, and O. Ghattas. Low rank saddle free Newton: Algorithm and analysis. *submitted*, 2020. https://arxiv.org/abs/2002.02881.

[22] Operator inference for data-driven, non-intrusive model reduction of dynamical systems. https://github.com/Willcox-Research-Group/rom-operator-inference-Python3.

[23] Benjamin Peherstorfer, Karen Willcox, and Max Gunzburger. Survey of multifidelity methods in uncertainty propagation, inference, and optimization. *SIAM Review*, 60(3):550–591, 2018.

[24] Teresa Portone, Damon McDougall, and Robert D Moser. A stochastic operator approach to model inadequacy with applications to contaminant transport. *arXiv preprint arXiv:1702.07779*, 2017.

[25] Byung-Jun Yoon, Xiaoning Qian, and Edward R. Dougherty. Quantifying the multi-objective cost of uncertainty, 2020.

[26] J. Zech and Y. M. Marzouk. Sparse approximation of triangular transports on bounded domains. *arXiv:2006.06994, submitted*, 2020.

[27] Guang Zhao, Xiaoning Qian, Byung-Jun Yoon, Francis J Alexander, and Edward R Dougherty. Model-based robust filtering and experimental design for stochastic differential equation systems. *IEEE Transactions on Signal Processing*, 68:3849–3859, 2020.

[28] Guang Zhao, Xiaoning Qian, Byung-Jun Yoon, Francis J Alexander, and Edward R Dougherty. Bayesian active learning by soft mean objective cost of uncertainty. submitted.

[29] Guang Zhao, Xiaoning Qian, Byung-Jun Yoon, Francis J Alexander, and Edward R Dougherty. Uncertainty-aware active learning for optimal Bayesian classifier. submitted.

A. Organizational chart

DRIVING SCIENTIFIC APPLICATION AREA: ADVANCED MANUFACTURING & MATERIALS	
additive manufacturing testbed (Turner)	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 3: 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 2 of the center (September 2019–September 2020), their positions and institutional affiliations, and the percentage of their time dedicated to each one of the major AEOLUS research tasks.

AEOLUS WORK BREAKDOWN STRUCTURE -- YEAR 2

	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	40		30	25	0			5	100
Yuanxun Bao, UT postdoc	80			20	0				100
Yigong Qin, UT PhD student	100		0	0					100
Omar Ghattas, UT PI and center co-director	5	10	15	15	15	15	5	20	100
Peng Chen, UT research associate		10	20	20	20	20	10		100
Nick Alger, UT postdoc			50	50					100
Amal Alghamdi, UT postdoc			50	50					100
Josh Chen, UT PhD student		20	50	20			10		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
Teresa Portone, UT PhD student							100		100
J. Tinsley Oden, UT co-PI	10	40	5		15		30		100
Danial Faghihi, UT research associate, now assistant professor, U. of Buffalo	25	20	10	5		25	15		100
Lianghao Cao, UT PhD student	10	70			20				100
Prashant Jha, postdoc	10	70	10			10			100
Karen Willcox, UT PI and center co-director	10		20	40	10			20	100
Parisa Khodabakhshi, UT postdoc	30			70					100
Rudy Geelen, UT postdoc	10			90					100
Sean McBane, UT PhD student	10			50	40				100
Shane McQuarrie, UT PhD student			10	90					100
Youssef Marzouk, MIT co-PI		10	50			30		10	100
Jakob Zech, MIT postdoc			100						100
Ricardo Baptista, MIT PhD student		10	50			40			100
Robert Ren, MIT PhD student			100						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
Clayton Webster, UTK PI		20	20	40	5	5		10	100
Max Gunzburger, UT Senior Researcher	30	20	10	30	10				100
John Turner, ORNL PI	50							50	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		35	35			100
Omar Maddouri, TAMU PhD student			50		50				100
Guang Zhao, TAMU PhD student			50			50			100

C. AEOLUS publications, September 2019–September 2020

C.1. Publications appeared or accepted

1. N. Alger, P. Chen, O. Ghattas, Tensor train construction from tensor actions, with application to compression of large high order derivative tensors, SIAM Journal on Scientific Computing, to appear, 2020. https://arxiv.org/abs/2002.06244

2. A. Alghamdi, M. Hesse, J. Chen, O. Ghattas, Bayesian Poroelastic Aquifer Characterization from InSAR Surface Deformation Data. Part I: Maximum A Posteriori Estimate, Water Resources Research, 56:e2020WR027391, 2020. https://doi.org/10.1029/2020WR027391

3. I. Ambartsumyan, W. Boukaram, T. Bui-Thanh, O. Ghattas, D. Keyes, G. Stadler, G. Turkiyyah, and S. Zampini, Hierarchical Matrix Approximations of Hessians Arising in Inverse Problems Governed by PDEs, SIAM Journal on Scientific Computing, to appear, 2020. http://arxiv.org/abs/2003.10173

4. M. Andreas, S. Bakas, S. Subramanian, C. Davatzikos, and G. Biros, Integrated Biophysical Modeling and Image Analysis: Application to Neuro-Oncology, Annual Review of Biomedical Engineering, 22, pp. 309–341, 2020 https://doi.org/10.1146/annurev-bioeng-062117-121105

5. D Agarwal, G Biros. Stable shapes of three-dimensional vesicles in unconfined and confined Poiseuille flow. Physical Review Fluids 5 (1), 013603. https://link.aps.org/pdf/10.1103/PhysRevFluids.5.013603

6. Bardsley, J., Cui, T., Marzouk, Y.M., Wang, Z. Scalable optimization-based sampling on function space. SIAM Journal on Scientific Computing 42: A1317–1347 (2020).

7. 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, to appear, 2020.

8. G Biros, U Meier Yang. Proceedings of the 2020 SIAM Conference on Parallel Processing for Scientific Computing. Society for Industrial and Applied Mathematics. https://epubs.siam.org/doi/abs/10.1137/1.9781611976137

9. Brennan, M., Bigoni, D., Zahm, O., Spantini, A., Marzouk, Y.M. Greedy inference with structure-exploiting lazy maps. Advances in Neural Information Processing Systems (NeurIPS) 2020. Selected for oral presentation. https://arxiv.org/abs/1906.00031

10. O. Burkovska and M. Gunzburger, Affine Approximation of Parametrized Kernels and Model Order Reduction for Nonlocal and Fractional Laplace Models, SIAM Journal on Numerical Analysis 58 (3), 1469-1494, May 2020. https://epubs.siam.org/doi/10.1137/19M124321X

11. Cabrera, J. M., Moser, R. D., and Ezekoye, O. A. 2020 A Modified Directional Flame Thermometer: Development, Calibration, and Uncertainty Quantification. Journal of Verification, Validation and Uncertainty Quantification, 5(1), 011003.

12. Cabrera, J.-M., Moser, R. D. and Ezekoye, O. A. 2019 A Bayesian Method for Determining the Fire Evolution Within a Compartment, ASTFE Digital Library. Begel House Inc., 2019.

13. G. Capodaglio, M. Gunzburger, and H. Wynn, Approximation of probability density functions for PDEs with random parameters using truncated series expansions. To appear in a special issue of

the Vietnam Journal of Mathematics dedicated to Prof. Enrique Zuazua on the occasion of his 60th birthday, 2020

14. G. Capodaglio, M. D'Elia, P. Bochev, and M. Gunzburger, An energy-based coupling approach to nonlocal interface problems, Computers & Fluids, 207, 2020.

15. P. Chen and O. Ghattas, Projected Stein variational gradient descent, NeurIPS 2020, to appear, December 2020. https://arxiv.org/abs/2002.03469

16. N. Dexter, H. Tran, and C. G. Webster. Reconstructing high-dimensional Hilbert-valued functions via compressed sensing. In 13th International conference on Sampling Theory and Applications SampTA, pages 1–5, Bordeaux, France, 2019.

17. N. Dexter, H. Tran, and C. G. Webster. A mixed ℓ_1 regularization approach for sparse simultaneous approximation of parameterized PDEs. M2N: Mathematical Modelling and Numerical Analysis, 53(6):2025–2045, 2019.

18. D. Faghihi, X. Feng, E.A.B.F. Lima, J.T. Oden, and T. E. Yankeelov. A Coupled Mass Transport and Deformation Theory of Multi-constituent tumor Growth, Journal of the Mechanics and Physics of Solids, v. 139, p 103936, June 2020. https://doi.org/10.1016/j.jmps.2020.103936

19. D. Faghihi, D.; K. Ravi-Chandar, and J. T. Oden. A Stochastic Dynamic Data-Driven Framework for Real-time Prediction of Materials Damage in Composites, Dynamic Data Driven Application Systems II, Edited by F. Darema, Lecture Notes in Computer Science, Springer, (in press 2020).

20. Faghihi, D., Carey, V., Michoski, C., Hager, R., Janhunen, S., Chang, C. S., and Moser, R. D. 2020 Moment preserving constrained resampling with applications to particle-in-cell methods. Journal of Computational Physics, 409, 109317.

21. Marvin Fritz, E.A.B.F. Lima, Vanja Nikolic, J.T. Oden, and B. Wohlmuth. Local and Nonlocal Phase-Field Models of Tumor Growth and Invasion Due to ECM Degradation, M3AS (Mathematical Models and Methods in Applied Sciences), v. 29, no. 13, pp. 2433-2458, October 2019. https://doi.org/10.1142/S0218202519500519

22. David Fuentes, J.T. Oden, K. Diller, J. Yung, Y. Feng, J.D. Hazle, A. Shetty, and R. J. Stafford. Computational and Magnetic Resonance -guided Patient-Specific Laser Induced Thermal Therapy of Cancer, Dynamic Data Driven Application Systems II, Edited by F. Darema, Lecture Notes in Computer Science, Springer, (in press 2020).

23. Haering, S., Oliver, T. A. and Moser, R. D. 2019 Towards a Predictive Hybrid RANS/LES Framework, AIAA Scitech 2019 Forum.

24. Haering, S. W., Lee, M., and Moser, R. D. 2019 Resolution-induced anisotropy in large-eddy simulations. Physical Review Fluids, 4(11), 114605.

25. Prashant K. Jha, Lianghao Cao, and J. Tinsley Oden. Bayesian-based predictions of COVID-19 evolution in Texas using multispecies mixture-theoretic continuum models. Computational Mechanics (2020): 1-14.

26. Ustim Khristenko, Andrei Constantinescu, Patrick Le Tallec, J. Tinsley Oden, and Barbara Wohlmuth. A Statistical Framework for Generating Microstructures of Two-Phase Random Materials: Application to Fatigue Analysis, Multiscale Modeling and Simulation, v. 18, no. 1, pp. 21-43, 2020. https://doi.org/10.1137/19M1259286.

27. Kramer, B., and Willcox, K., Balanced Truncation Model Reduction for Lifted Nonlinear Systems. In Realization and Model Reduction of Dynamical Systems, Springer, to appear, 2020.

28. Lee, M and Moser, R. D. 2019 Spectral analysis of the budget equation in turbulent channel flows at high Reynolds number, J. Fluid Mech. 860, 886-938.

29. G. Lorenzo, D. Hormuth II, A. Jarrett, E.A.B.F. Lima, S. Subramanian, G. Biros, J.T. Oden, T.J.R. Hughes, and T.E. Yankeelov. Quantitative in vivo Imaging to Enable Tumor Forecasting and Optimization of Therapeutic Response in Cancer, Complexity, Computation, part of Springer series: Emergence, Complexity, Computation, Zelinka, I. (Ed), Adamatzky, A. (Ed), Chen, G. (Ed) (in press 2020)

30. Oliver, T. A, Bogard, D. D. and Moser, R. D. 2019 Large eddy simulation of compressible, shaped-hole film cooling, Int. J. Heat and Mass Transfer 140, 498-517.

31. A. Petrosyan, A. Dereventsov, and C. G. Webster. Neural network integral representations with the ReLU activation function. Proceedings of Machine Learning Research, 2020. Accepted https://arxiv.org/abs/1910.02743

32. A. Petrosyan, H. Tran, and C. G. Webster. Reconstruction of jointly sparse vectors via manifold optimization. Applied Numerical Mathematics, 144:140–150, 2019.

33. Qian, E., Kramer, B., Peherstorfer, B., and Willcox, K., Lift & Learn: Physics-informed machine learning for large-scale nonlinear dynamical systems. Physica D: Nonlinear Phenomena, Volume 406, May 2020, 132401.

34. V. Reshniak, J. Trageser, and C. G. Webster. A nonlocal feature-driven exemplar-based approach for image inpainting. SIAM Journal on Imaging Sciences, 2020. Accepted https://arxiv.org/abs/1909.09301

35. K. Scheufele, S. Subramanian, and G. Biros, Fully Automatic Calibration of Tumor-Growth Models Using a Single mpMRI Scan, IEEE Transactions on Medical Imaging, 2020. https://doi.org/10.1109/TMI.2020.3024264

36. K. Scheufele, S. Subramanian, A. Mang, G. Biros, and M. Mehl, Image- Driven Biophysical Tumor Growth Model Calibration, SIAM Journal on Scientific Computing, 2020. https://doi.org/10.1137/19M1275280

37. S Subramanian, K Scheufele, M Mehl, G Biros. Where did the tumor start? An inverse solver with sparse localization for tumor growth models. Inverse Problems 36 (4), 045006. https://iopscience.iop.org/article/10.1088/1361-6420/ab649c/meta

38. Swischuk, R., Kramer, B., Huang, C., and Willcox, K., Learning physics-based reduced-order models for a single-injector combustion process. AIAA Journal, Vol. 58, No. 6, June 2020, pp. 2658-2672. Also in Proceedings of 2020 AIAA SciTech Forum & Exhibition, Orlando FL, January, 2020.

39. Tong, X. T., Morzfeld, M., Marzouk, Y.M. MALA-within-Gibbs samplers for high-dimensional distributions with sparse conditional structure. SIAM Journal on Scientific Computing 42: A1765–A1788 (2020).

40. H. Tran and C. G. Webster. A class of null space conditions for sparse recovery via nonconvex, non-separable minimizations. Results in Applied Mathematics, 3:100011, 2019.

41. Wu, C., Hormuth, D. A., Oliver, T. A., Pineda, F., Lorenzo, G., Karczmar, G. S., Moser, R. D. and Yankeelov, T. E. 2020 Patient-Specific Characterization of Breast Cancer Hemodynamics Using Image-Guided Computational Fluid Dynamics. IEEE Transactions on Medical Imaging 39(9), 2760-2771.

42. X. Xie, C. G. Webster, and T. Iliescu. Closure Learning for Nonlinear Model Reduction Using Deep Residual Neural Network. Fluids, 5(1,39):1–15, 2020.

43. X. Xie, G. Zhang, and C. G. Webster. Non-intrusive inference reduced order model for fluids using deep multistep neural network. Mathematics, 7(8):1–15, 2019.

44. Guang Zhao, Xiaoning Qian, Byung-Jun Yoon, Francis J. Alexander, and Edward R. Dougherty, Model-based robust filtering and experimental design for stochastic differential equation systems, IEEE Transactions on Signal Processing, vol. 68, 3849-3859, 2020.

C.2. Publications submitted

1. R. Baptista, O. Zahm, Y. M. Marzouk. An adaptive transport framework for joint and conditional density estimation. Preprint (2020). https://arxiv.org/abs/2009.10303

2. Shahin Boluki, Xiaoning Qian, Edward R Dougherty. Optimal Bayesian supervised domain adaptation for RNA sequencing data, Bioinformatics, 2020 (submitted).

3. M Brunn, N Himthani, G Biros, M Mehl, A Mang. Multi-Node Multi-GPU Diffeomorphic Image Registration for Large-Scale Imaging Problems. https://arxiv.org/abs/2008.12820

4. M Brunn, N Himthani, G Biros, M Mehl, A Mang. Fast GPU 3D Diffeomorphic Image Registration. https://arxiv.org/abs/2004.08893

5. O. Burkovska and M. Gunzburger, On a nonlocal Cahn-Hilliard model permitting sharp interfaces. Submitted, April 2020. https://arxiv.org/abs/2004.14379

6. O. Burkovska, C. Glusa, and M. D'Elia, An optimization-based approach to parameter learning for fractional type nonlocal models. Submitted, Oct. 2020. https://arxiv.org/abs/2010.03666

7. P. Chen, M.R. Haberman, and O. Ghattas, Optimal design of acoustic metamaterial cloaks under uncertainty, submitted, 2020. https://arxiv.org/abs/2007.13252

8. P. Chen, O. Ghattas, Stein variational reduced basis Bayesian inversion, submitted, 2020. http://arxiv.org/abs/2002.10924

9. J. Daws, A. Petrosyan, H. Tran, and C. G. Webster. A Weighted l1-minimization approach for wavelet reconstruction of signals and images. IEEE Transactions on Signal Processing, 2019, submitted. https://arxiv.org/abs/1909.07270

10. A. Dereventsov, C. G. Webster, and J. Daws. An adaptive stochastic gradient-free approach for high-dimensional blackbox optimization. In Advances in Neural Information Processing Systems 32. Curran Associates, Inc., 2020. Submitted. https://arxiv.org/abs/2006.10887

11. A. Dereventsov and C. G. Webster. The Natural Greedy Algorithm for reduced bases in Banach spaces. Foundations of Computational Mathematics, 2019, submitted. https://arxiv.org/abs/1905.06448

12. 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, 2020, under review in Nonlinear Analysis: Real World Applications. https://arxiv.org/abs/2006.10477

13. Youngjoon Hong, Bongsuk Kwon, Byung-Jun Yoon, Optimal experimental design for uncertain systems based on coupled differential equations, submitted to IEEE Signal Processing Letters. https://arxiv.org/abs/2007.06117

14. Kovachki, N., Baptista, R., Hosseini, B., Marzouk, Y. M. Conditional sampling with monotone GANs, preprint (2020). https://arxiv.org/abs/2006.06755

15. T. O'Leary-Roseberry and O. Ghattas, Ill-posedness and optimization geometry for nonlinear neural network training, submitted, 2020. https://arxiv.org/abs/2002.02882

16. T. O'Leary-Roseberry, N. Alger, and O. Ghattas, Low rank saddle free Newton: Algorithm and analysis, submitted, 2020. https://arxiv.org/abs/2002.02881

17. Y. Xu, A. Narayan, H. Tran, and C. G. Webster. Analysis of the ratio of l1 and l2 norms in compressed sensing. Applied and Computational Harmonic Analysis, 2020, submitted. https://arxiv.org/abs/2004.05873

18. C. Vollman, M. D'Elia, and M. Gunzburger, A cookbook for finite element methods for nonlocal problems, including quadrature rules and approximate Euclidean balls, submitted, 2020. https://arxiv.org/abs/2005.10775

19. Yoon, B-J, Qian, X, and E. R. Dougherty, Quantifying the Multi-objective Cost of Uncertainty, submitted to IEEE Signal Processing Letters.

20. Zech, J., Marzouk, Y. M. Sparse approximation of triangular transports on bounded domains. Submitted to Constructive Approximation (2020). https://arxiv.org/abs/2006.06994

21. Guang Zhao, Edward R. Dougherty, Byung-Jun Yoon, Francis J. Alexander, and Xiaoning Qian, Uncertainty-aware Active Learning for Optimal Bayesian Classifier, International Conference on Learning Representations (ICLR), 2021. (submitted)

22. Zhao, G., X. Qian, Alexander, F., and E. R. Dougherty, Bayesian Active Learning by Soft Mean Objective Cost of Uncertainty, submitted to AISTATS, 2021.

D. AEOLUS invited presentations, October 2019–October 2020

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

- Willcox gives a keynote invited talk "Predictive data science: From model reduction to scientific machine learning" at the INFORMS Annual Meeting, Seattle, WA, October 2019.

- Willcox gives an invited keynote talk "Predictive data science: From model reduction to scientific machine learning" at SC19, Denver, CO, November 2019 .

- Willcox gives an invited keynote lecture "Big Decisions need more than just Big Data" at the 23rd International Conference on Modelling and Simulation (MODSIM), Canberra, Australia, December 2019.

- Marzouk was scheduled to give an invited plenary talk at the SIAM Conference on Uncertainty Quantification (UQ20), Munich, Germany, March 2020. (cancelled due to COVID-19)
- O. Ghattas, Peruvian Conference on Scientific Computing, Cusco, Peru, March 30–April 2, 2020. (Plenary talk, Postponed)
- Willcox is scheduled to give an invited plenary talk at "Toward predictive digital twins: Component-based adaptive reduced-order models and interpretable machine learning." at the World Congress on Computational Mechanics (WCCM), July 2020. (This conference was postponed to January 2021.)
- Willcox gives an invited plenary talk "Predictive digital twins: Where data-driven learning meets physics-based modeling" at JuliaCon, July 2020.
- Willcox gives the opening keynote lecture "Toward predictive digital twins: From physics-based modeling to scientific machine learning" at the ASME Design Automation Conference, August 2020.
- Ghattas gives an invited plenary lecture "Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems and optimal experimental design" at the Opening Conference, NSF Institute for Mathematics and Statistics Innovation, University of Chicago, October 7–9, 2020.
- Willcox gives an invited plenary lecture "Toward predictive digital twins: From physics-based modeling to scientific machine learning" at the Opening Conference, NSF Institute for Mathematics and Statistics Innovation, University of Chicago, October 7–9, 2020.

D.2. Other invited conference and workshop talks

- G. Biros, Operator-splitting ROMs for problems with moving interfaces, ICERM workshop on Computational Statistics and Data-Driven Models, Brown University (virtual), April 20–24, 2020.
- O. Burkovska, On some nonlocal diffusion problems with inequality constraints, Department of Mathematics, University of Tennessee, Knoxville, February 5, 2020 (Invited seminar talk)
- O. Burkovska, 50th Barrett Memorial Lectures, Approximation, Applications, and Analysis of Nonlinear Nonlocal Models, University of Tennessee, Knoxville, May 11-13, 2020 (Invited speaker, Postponed to 2021)
- O. Burkovska, On the properties of the nonlocal Cahn-Hilliard model with the double obstacle potential, RICAM Special Semester on Optimization, Optimal Control and Optimization for Nonlocal Models, Linz, Austria. Oct. 28-30, 2020 (Invited talk)
- O. Ghattas Parsimonious structure-exploiting deep neural network surrogates for Bayesian inverse problems, Society for Engineering Science, 2020 Virtual Technical Meeting, September 29–October 1, 2020. (Invited)
- O. Ghattas, Fast methods for Bayesian inverse problems governed by stochastic PDEs, World Congress on Computational Mechanics, Paris, France, July 19–24, 2020. (Invited, Postponed)
- O. Ghattas, Computational Uncertainty Quantification: Mathematical Foundations, Methodology, and Data, Erwin Schrödinger International Institute for Mathematics and Physics, Vienna, Austria, May 11–15, 2020. (Invited, Postponed)

- O. Ghattas, Optimal neural networks for learning high-dimensional input-output maps defined by PDEs, SIAM Conference on Mathematics of Data Science, May 5–8, 2020. (Invited, Cancelled)
- O. Ghattas, Oberwolfach Workshop on Data Assimilation, Oberwolfach, Germany, April 12–18, 2020. (Invited, Cancelled)
- O. Ghattas, SIAM Conference on Uncertainty Quantification, Munich, Germany, March 24–27, 2020. (Invited, Cancelled)
- O. Ghattas, Machine Learning for Inferring Scientific Models: Hope or Hype? NSF Workshop on Artificial Intelligence in Natural Hazards Engineering, Austin, TX, February 18–19, 2020. (invited)
- O. Ghattas, Machine Learning for Inferring Scientific Models: Hope or Hype?, Shell, Houston, TX, January 29, 2020. (invited)
- O. Ghattas, Scalable Methods for Bayesian Optimal Experimental Design, International Workshop on Data-Centric Engineering, Cambridge, MA, December 9–12, 2019. (invited)
- O. Ghattas, Fast methods for Bayesian inverse problems governed by random PDE forward models, Workshop on Optimization and Inversion under Uncertainty, Radon Institute for Computational and Applied Mathematics (RICAM) of the Austrian Academy of Sciences, Linz, Austria, November 11–15, 2019. (Invited)
- O. Ghattas, Scalable Optimal Experimental Design for Bayesian Inverse Problems, Workshop on Big Data, Data Assimilation, and Uncertainty Quantification, Institut Henri Poincare, Paris, France, November 12–15, 2019. (Invited)
- O. Ghattas, Optimal Experimental Design for Large-Scale Bayesian Inverse Problems via Multi-PDE-Constrained Optimization, Workshop on New Trends in PDE-Constrained Optimization, Radon Institute for Computational and Applied Mathematics (RICAM) of the Austrian Academy of Sciences, Linz, Austria, October 14–18, 2019. (invited)
- P. Khodabakhshi, Nonlinear model reduction for one-dimensional solidification in additive manufacturing, GAMM Junior's Summer School on Applied Mathematics and Mechanics (SAMM) on Learning Models from Data: Model Reduction, System Identification and Machine Learning, July 2020.
- P. Khodabakhshi, Data driven reduced order model for solidification process in additive manufacturing, Model Order Reduction Summer School 2020 at EPFL, September 2020.
- Y. Marzouk, ExxonMobil Upstream Research Company. Houston, TX, October 2019.
- Y. Marzouk, RWTH-Aachen University, School for Simulation and Data Science seminar. Aachen, Germany, October 2019.
- Y. Marzouk, Universität Heidelberg, Department of Mathematics. Heidelberg, Germany, October 2019.
- Y. Marzouk, California Institute of Technology, Computing + Mathematical Sciences. Pasadena, CA, February 2020.
- Y. Marzouk, Optimal Transport: Advances and Applications. Keynote speaker. Cambridge, MA, May 2020. (cancelled due to COVID-19)

- Y. Marzouk, Bernoulli-IMS 10th World Congress on Probability and Statistics. Invited session speaker. Seoul, Korea, August 2020. (Now postponed to July 2021, due to COVID-19)
- R. Moser, Exploiting Synergies Between RANS and LES Representations of Turbulence: Rethinking Hybrid Modeling, Stanford University, February, 2020.
- R. Moser, Computation as a Tool of Fluid Dynamics Engineering and Research, Vanderbilt University, February, 2020.
- R. Moser, Investigating Wall-Bounded Turbulence in Direct Numerical Simulations, Harvard Univer- sity, November, 2019.
- R. Moser, Investigating Wall-Bounded Turbulence in Direct Numerical Simulations, Arizona State University, October 2019.
- J.T. Oden Computational Models of the Growth of Vascular Tumors Embedded in an Evolving Capillary Network, presented at the Virtual Technical Meeting of the Society of Engineering Science 2020, Eringen Medal Symposium honoring Professor Thomas J.R. Hughes, held September 28-29, 2020.
- S. Subramanian, MRI-driven Inverse Problems for Brain Tumor Growth Models in Personalized Medicine, SIAM Texas-Louisiana Section Annual Meeting, South Methodist University, Dallas, November 2019.
- K. Willcox, Multifidelity uncertainty quantification for optimization under uncertainty. Invited Plenary Lecture. Workshop on Uncertainty Quantification, The Australian National University, November 2019.
- K. Willcox, Data-centric engineering: From physics-based models to scientific machine learning. Invited talk, International Workshop on Data-Centric Engineering, Cambridge, MA, December 2019.
- K. Willcox, A technology roadmap towards Digital Thread. Invited talk, Panel on Multidisciplinary Design Optimization & Model-based Systems Engineering, AIAA Scitech Forum, Orlando, FL, January 2020
- K. Willcox, Toward predictive digital twins via component-based reduced-order models and interpretable machine learning. Invited talk, Institute of High Performance Computing, A*STAR, Singapore, January 2020.
- K. Willcox, Challenges and progress in learning physics-based reduced models for combustion processes. Invited plenary talk, Workshop on Exuberance of Machine Learning in Transport Phenomena, Dallas, TX, February 2020.
- K. Willcox, Predictive data science: From physics-based models to scientific machine learning. Shell Lecture (invited), Rice University, February 2020.
- K. Willcox, Predictive Digital Twins & Multifidelity Modeling. Invited talk, Lockheed Martin Aeronautics, Dallas, TX, February 2020.
- K. Willcox, Predictive data science: From physics-based models to scientific machine learning. Invited talk, ICERM Workshop on the Mathematics of Model Reduction, Providence, RI, February 2020.

- K. Willcox, Towards Predictive Data Science: From Scientific Machine Learning to Digital Twins. Keynote talk, Women in Data Science (WiDS) Conference, Austin, TX, March 2020.
- K. Willcox, Scientific Machine Learning: Where physics-based modeling meets data-driven learning. Santa Fe Institute Colloquium, May 2020.
- K. Willcox, Predictive digital twins: Where data-driven learning meets physics-based modeling. Workshop on Learning for Dynamics and Control (L4DC), June 2020.
- K. Willcox, Computing Needs for Digital Twins: Where physics-based modeling meets data-driven learning. Keynote talk, NASA High-End Computing Workshop, June 2020.
- K. Willcox, Predictive digital twins: Where dynamic data-driven learning meets physics-based modeling. Keynote Talk, DDDAS2020, October 2020.
- K. Willcox, The future needs Computational Science and Engineering. Keynote Talk, Altair Technology Conference, October 2020.

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 and laboratory positions.

E.1. Software

- hIPPYlib: Inverse Problem PYthon library (https://hippylib.github.io/). 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.
- Operator Inference model reduction package with tutorial examples. Released June 2020. https://github.com/Willcox-Research-Group/rom-operator-inference-Python3
- Python code for Kuramoto model OED (optimal experimental design) simulations in GitHub: https://github.com/yhong2/Sync
- Matlab code for robust filtering and OED with stochastic differential equations (SDEs): https://github.com/QianLab/SDE-MOCU
- MUQ: MIT Uncertainty Quantification Library: http://muq.mit.edu
- MIT TransportMaps library: http://transportmaps.mit.edu

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

- Ghattas was organizer and instructor for the short course on Inverse Problems and Uncertainty Quantification, Trimester on Mathematics of Climate and the Environment, Institut Henri Poincaré, Paris, France, November 4–8, 2019.
- Webster taught the short course on Uncertainty Quantification and Approximation Theory for Parameterized PDEs, School of Mathematics, African Institute for Mathematical Sciences (AIMS), Cape Town, South Africa, September 2019.

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.

- Frank Alexander, Omar Ghattas and Karen Willcox are on the Program Committee for the New York Scientific Data Summit 2020, October 20–23, 2020. https://www.bnl.gov/nysds20/
- The Oden Institute and Sandia National Laboratories co-host an abbreviated virtual Rising Stars in Computational & Data Sciences in October 2020, bringing 32 outstanding female PhD students and postdocs together for a half-day virtual workshop.
- Biros and Ghattas are co-organizers, Workshop on Future Directions in Extreme Scale Computing for Scientific Grand Challenges, Texas Advanced Computing Center, Austin, TX, January 9–10, 2020.
- Ghattas and Marzouk are co-organizers, Workshop on Mathematical Foundations of Data Assimilation and Inverse Problems, Foundations of Computational Mathematics (FoCM'20), Vancouver, Canada, June 15-24, 2020. [Cancelled]
- Ghattas is co-organizer, Workshop on Mathematical Modeling in Glaciology, Banff International Research Station, Banff, Canada, January 12–17, 2020.
- Ghattas is co-organizer, Workshop on Big Data, Data Assimilation, and Uncertainty Quantification, Trimester on Mathematics of Climate and the Environment, Institut Henri Poincaré, Paris, France, November 12–15, 2019.
- Ghattas is on the Scientific Committee, Conference on Uncertainty Quantification in Computational Sciences and Engineering (UNCECOMP 2021), Athens, Greece, June 21–23, 2021.
- Ghattas was on the Scientific Committee, 14th World Congress in Computational Mechanics and ECCOMAS Congress 2020, Paris, France, July 19–24, 2020.
- Ghattas was on the International Organizing Committee (IOC), 5th International Symposium on Inverse Problems, Design, and Optimization (IPDO2019), Tianjin, China, September 24–26, 2019.
- Marzouk serves as co-chair of organizing committee, 2021 SIAM Conference on Mathematical and Computational Issues in the Geosciences (SIAM GS21)
- Marzouk serves on the Scientific Committee, 16th US National Congress on Computational Mechanics (USNCCM-16)
- Webster is co-chair of the ICERM Workshop on Safety and Security of Deep Learning, ICERM, Brown University, 2021.
- Webster is chair of the 2019 SIAM SEAS Annual Conference, The University of Tennessee, Knoxville, TN.
- Webster is a member of the Scientific Committee for the 8th workshop on high-dimensional approximation, Seminar for Applied Mathematics, ETH Zurich, Zurich, Switzerland.
- Willcox served on the Copper Mountain Conference 2020 Organizing Committee.

- Willcox serves on the Organizing Committee, International Congress on Industrial and Applied Mathematics (ICIAM) 2023
- Willcox is a member of the Scientific Committee for ECCOMAS Conference Math 2 Product 2021

E.4. Other notable professional activities

- 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 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 serves as Chair, SIAM Activity Group on Uncertainty Quantification, 2019–2020
- Marzouk serves on the Advisory Board, UK EPSRC Computational Statistical Inference for Engineering and Security (CoSInES) program
- J. Tinsley 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 serves 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 is elected to the Board of Trustees of the American Institute of Aeronautics and Astronautics (AIAA), 2020–2023
- Willcox serves on the Board of Trustees of the new Institute for Mathematics and Statistics Innovation, 2020–
- Willcox serves as inaugural Program Director, SIAM Activity Group on Data Science, 2020–2021