Final Report

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DiaMonD: An Integrated Multifaceted Approach to Mathematics at the Interfaces of Data, Models, and Decisions

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The major goal of the project was to invent, analyze, implement, and apply new algorithms to speed up the computational simulation of complex systems in settings in which multiple simulations are needed. The main efforts we undertook are as follows.

1. Develop novel reduced order methods to reduce the costs of simulations, especially in settings (e.g., UQ, inference, optimization and control) for which numerous simulation are needed and also for nonlocal problems (e.g., fractional derivative, anomalous diffusion, nonlocal mechanics) for which lack of sparsity results in more expensive full-order simulation than encountered in partial differential equations settings; rigorous analyses as well as computational tests were carried out.

2. Develop multifidelity methods based on the usage of a variety of models having different fidelities and different costs to accelerate simulations again in settings where numerous simulations are needed or are especially expensive; rigorous analyses as well as computational tests were carried out.

3. Develop ensemble methods to reduced the costs of simulations again in settings where numerous simulations are needed or are especially expensive; rigorous analyses as well as computational tests were carried out.

4. Analyze a model for Richardson pair dispersion in turbulent flows and develop discretization methods for the efficient and accurate approximations of the solution of the model; rigorous analyses as well as computational tests were carried out.

In the following sections we discussed each of these efforts, after which we list the products produced reporting on our efforts. For each of the four efforts listed above, details about the efforts are found in the products cited for each effort.

[1]Lead institutions: The University of Texas at Austin and the Massachusetts Institute of Technology. PIs: Omar Ghattas and Karen Willcox

1. ***Reduced-order modeling*** [1,2,3,4,6,9,13,14]

with senior investigators: Donald Estep (Colorado State U), Janet Peterson (FSU), Clayton Webster (ORNL), Guannan Zhang (ORNL)

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An efficient parameter space domain decomposition reduced-order modeling method and a posteriori error estimation

Efficient algorithms were developed for a reduced-order model based on the proper orthogonal decomposition methodology for the solution of parameterized elliptic partial differential equations. The method relies on partitioning the parameter space into subdomains based on the properties of the solution space and then forming a reduced basis for each of the subdomains. This yields more efficient offline and online stages for the proper orthogonal decomposition method. We extended these ideas to the task of inexpensive adjoint based a posteriori error estimation of both the expensive finite element method solutions and the reduced-order model solutions, for single and multiple quantities of interest. Rigorous analyses were used to justify claims made about the new methodology and also to guide the selection of parameters that appear in the algorithms. Several numerical results illustrated the efficacy of the approach.

Ensemble-proper orthogonal decomposition method for the nonstationary Navier-Stokes equations

Many partial differential equations (PDE) are described in terms of parameters, such as viscosity or density. An analysis of the PDE may involve considering a large range of parameter values, as occurs in uncertainty quantification, collocation, and various statistical techniques. The solution of even a single case may be quite expensive; while parallel computing may be applied, this reduces the total elapsed time but not the total computational effort. We consider the case of the time-dependent Navier-Stokes equations for which a recently developed ensemble-based method[2] allows for the efficient determination of the multiple solutions corresponding to many parameter sets. The method uses the average of the multiple solutions at any time step to define a linear set of equations that determines the solutions at the next time step. To significantly further reduce the costs of determining multiple solutions of the Navier-Stokes equations, we incorporate a proper orthogonal decomposition (POD) reduced-order model into the ensemble-based method. Stability and convergence results for first- and higher-order accurate ensemble-POD methods are were obtained. Numerical experiments illustrate the accuracy and efficiency of this approach.

A Leray regularized ensemble-proper orthogonal decomposition method for parameterized convection-dominated flows

Partial differential equations (PDEs) are often dependent on input quantities which are uncertain. To quantify this uncertainty, PDEs must be solved over a large ensemble of parameters. Even for a single realization this can a computationally intensive process. In the case of flows governed by the Navier-Stokes equations, an efficient method has been devised for computing an ensemble of solutions. As discussed in the previous paragraph, to further reduce the computational cost of this method, an ensemble proper orthogonal decomposition (POD) method was recently developed. We then developed POD spatially filtered ensemble-POD methods so as to enhance the applicability of or approach to flows with higher Reynolds numbers. The POD spatial filter made it possible to construct a Leray ensemble-POD model, i.e., a regularized-reduced order model for

[2] A further discussion of ensemble based methods is given in Section 3.

the numerical simulation of convection-dominated flows. The Leray ensemble-POD model employs the POD spatial filter to smooth (regularize) the convection term in the Navier-Stokes equations and greatly diminishes the numerical inaccuracies produced by the ensemble-POD method in the numerical simulation of convection-dominated flows. Specifically, for the numerical simulation of a convection-dominated two-dimensional flow between two offset cylinders, we show that the Leray ensemble-POD method yields accurate results, whereas the unfiltered ensemble-POD is highly inaccurate. Error estimates for the novel Leray ensemble-POD algorithm are also proven.

Proper orthogonal decomposition and reduced-basis methods for nonlocal diffusion problems

In several application settings, diffusive behavior is observed to not follow the rate of spread predicted by parabolic partial differential equations (PDEs) such as the heat equation. Such behaviors, often referred to as anomalous diffusion, can be modeled using nonlocal (e.g., integral equations) in which points at a finite distance apart can interact. An example of such models is provided by fractional derivative equations. Because of the nonlocal interactions, discretized nonlocal systems have less sparsity, often significantly less, compared to corresponding discretized PDE systems. As such, the need for reduced-order surrogates which can be used to cheaply determine approximate solutions is much more acute for nonlocal models compared to that for PDEs.

We investigated the construction, application, and testing of proper orthogonal decomposition (POD) reduced-order models for an integral equation model for nonlocal diffusion. For certain modeling parameters, the model we consider allows for discontinuous solutions and includes, as a special case, fractional Laplacian kernels. Computational results illustrate the potential of using POD to obtain accurate approximations of solutions of nonlocal diffusion equations at much lower costs compared to, for example, standard finite element methods.

We also considered the construction, analysis, and application of reduced-basis methods for uncertainty quantification problems involving nonlocal diffusion problems with random input data. We developed reduced-basis approximations for nonlocal diffusion equations with affine random coefficients. Efficiency estimates of the proposed greedy reduced-basis methods were provided. Numerical examples were used to illustrate the effect that varying various model parameters have on the efficiency and accuracy of the reduced-basis method relative to sparse-grid interpolation using the full finite element method. It was shown that the proposed reduced-basis approach can indeed provide substantial savings while preserving sufficient accuracy compared to standard sparse-grid methods when combined with full finite element solvers.

Stabilized reduced-order models for the advection-diffusion-reaction equation using operator splitting

Reduced-order modeling coupled with finite element methods has been used effectively in many disciplines to efficiently solve complex problems. However, for advection-dominated flows numerical simulations often contain spurious, nonphysical oscillations which will also be apparent in the reduced order simulations. In this work, stabilization methods were developed for a reduced-order model for advection-diffusion-reaction equations when they are solved both with and without operator splitting. Specifically, the streamline-upwind Petrov Galerkin stabilization method and the spurious oscillations at layers diminishing stabilization method were considered. The stabilized reduced-order modeling results were compared numerically with their corresponding full finite element simulations, showing the efficacy of the reduced-order modeling approach with respect to accuracy per cost.

Algorithms and analyses for stochastic optimization for turbofan noise reduction using parallel reduced-order modeling

Simulation-based optimization of acoustic liner design in a turbofan engine nacelle for noise reduction purposes can dramatically reduce the cost and time needed for experimental designs. Because uncertainties are inevitable in the design process, we posed a stochastic optimization algorithm based on the conditional value-at-risk measure so that an ideal acoustic liner impedance is determined that is robust in the presence of uncertainties. A parallel reduced-order modeling framework was developed that dramatically improves the computational efficiency of the stochastic optimization solver for a realistic nacelle geometry. The reduced stochastic optimization solver takes less than 500 seconds to execute. In addition, well-posedness and finite element error analyses of the state system and optimization problem were proved and numerical illustrations were provided.

2. *Multifidelity methods for uncertainty quantification, optimization, and inference* [10,11,12]

with senior investigator: Karen Willcox (MIT)
postdoc: Benjamin Peherstorfer (MIT)]

In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, whereas lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Outer-loop applications, such as optimization, inference, and uncertainty quantification, require multiple model evaluations at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. The overall premise of the multifidelity methods we have developed is that low-fidelity models are leveraged for speedup whereas the high-fidelity model is kept in the loop to establish accuracy and/or convergence guarantees.

We first developed an optimal model management strategy that exploits multifidelity surrogate models to accelerate the estimation of statistics of outputs of computationally expensive high-fidelity models. Existing acceleration methods typically exploit a multilevel hierarchy of surrogate models that follow a known rate of error decay and computational costs; however, a general collection of surrogate models, which may include projection-based reduced models, data-fit models, support vector machines, coarser grid models, and simplified-physics models, does not necessarily give rise to such an explicit hierarchy. Our multifidelity approach provides a framework to combine an arbitrary number of surrogate models of any type. Instead of relying on error and cost rates, an optimization problem balances the number of model evaluations across the high-fidelity and surrogate models with respect to error and costs. We show that a unique analytic solution of the model management optimization problem exists under mild conditions on the models. Our multifidelity method makes occasional recourse to the high-fidelity model; in doing so it provides an unbiased estimator of the statistics of the high-fidelity model, even in the absence of error bounds and error estimators for the surrogate models. Numerical experiments with linear and nonlinear examples show that speedups by orders of magnitude are obtained compared to Monte Carlo estimation that only invokes a single high-cost, high-fidelity model.

We also investigated the properties of multifidelity Monte Carlo method we developed in the setting in which a hierarchy of approximations can be constructed with known error and cost bounds. Our main result is a convergence analysis of multifidelity Monte Carlo estimation, for which we prove a bound on the costs of the multifidelity Monte Carlo estimator under assumptions on

the error and cost bounds of the low-fidelity approximations. The assumptions we make are typical in the setting of similar Monte Carlo techniques. Numerical results were obtained to illustrate the derived theoretical bounds.

Our work on multifidelity methods culminated in a comprehensive survey, published in SIAM Review, of multifidelity methods that accelerate the solution of outer-loop applications by combining high-fidelity and low-fidelity model evaluations, where the low-fidelity evaluations arise from explicit low-fidelity models that approximates the same output quantity as the high-fidelity model. The review is broad in scope in that in addition to dealing with statistical estimation, it deals with applications in inference and optimization and also in that three multifidelity method strategies are considered: adaptation, fusion, and filtering.

3. *Ensemble methods for the efficient solution of flow problems* [3,4,6,7,8]

with FSU postdoc: Nan Jiang
FSU graduate student: Michael Schneier

In several important settings of computational fluid dynamics, a set of multiple simulations of a flow under different input conditions are required. Example of such settings include uncertainty quantification, reduced-order modeling, and optimization. The multiple approximate solutions of the Navier-Stokes equations could be generated from the use of different viscosity coefficients, initial conditions, and/or body forces. Due to the nonlinearity of the Navier-Stokes equations, straightforward linearization methods for the multiple simulations result in having not only different right-hand sides, but also different coefficient matrices. Following on work by William Layton and Nan Jiang, we have developed numerical algorithms for the efficiently determination of a set of such simulations. In the schemes, the average of the multiple solutions at any time step are used to construct multiple discrete systems all involving the same coefficient matrix but with different right-hand sides, and thus are computationally more efficient than solving for all the simulations separately. We developed two such schemes for both of which we showed that the schemes are nonlinearly and long-term stable under certain conditions on the time-step size and a parameter deviation ratio. Rigorous numerical error estimate showed that the two schemes are first-order and second-order accurate in time and optimally accurate in space. Several numerical experiments are presented to illustrate the theoretical results. Furthermore, we also developed a new numerical discretization of the variable viscosity ensemble algorithm in which the average viscosity is replaced with the maximum viscosity. It proved that this approach is significantly more stable than those in current use that use the average of the viscosity ensembles instead of the maximum value.

Additional work related to ensemble methods for the Navier-Stokes equations are discussed in Section 1 where these methods are combined with reduced-order modeling approaches.

4. *Simulation of Richardson pair dispersion in turbulent flows* [5]

with FSU postdoc: Nan Jiang
FSU graduate student: Feifei Xu

A fundamental problem in fluid flows is to determine the time history of the separation of two particles that are initially close together. For laminar flows, one expects that initially close particles remain close at later times, with the separation growing at most linearly in time. However, for turbulent flows, over long times the separation has been observed to grow faster than that, a phenomena knows as *Richardson pair dispersion,* with Richardson showing through dimensional

analysis arguments that the growth is proportional to t^3. To model this phenomena, we considered a turbulence closure model in which a fractional Laplacian of the velocity field is added to the Navier-Stokes equations to represent the turbulence diffusivity. We investigated the energy spectrum of the model and showed that only for the fractional Laplacian exponent $s = 1/3$ one obtains the Richardson t^3 growth in the particle separation. We then developed a modular time-stepping algorithm in semidiscretized form based on an operator splitting approach in which we decouple the standard Navier-Stokes operator from the fractional Laplacian modification term. In this way, the algorithm is minimally intrusive to a given legacy code for solving the NavierStokes equations. We prove that the algorithm is first-order accurate and unconditionally stable. We also derive error estimates for full discretizations of the model which, in addition to the time stepping algorithm, involves a finite element spatial discretization and a domain truncation approximation to the range of the fractional Laplacian.

Products

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[2] Q. Guan, M. Gunzburger, C. Webster, and G. Zhang; *Reduced basis methods for nonlocal diffusion problems with random input data*; Computer Methods in Applied Mechanics and Engineering **317** 2017, 746-770.

[3] M. Gunzburger, T. Iliescu, and M. Schneier; *A Leray regularized ensemble-proper orthogonal decomposition method for parameterized convection-dominated flows*; to appear in IMA Journal of Numerical Analysis.

[4] M. Gunzburger, N. Jiang, and M. Schneier; *An ensemble-proper orthogonal decomposition method for the nonstationary Navier-Stokes equations*; SIAM Journal on Numerical Analysis **55** 2017, 286-304.

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[7] M. Gunzburger, N. Jiang, and Z. Wang; *An efficient algorithm for simulating ensembles of parameterized flow problems*; to appear in IMA Journal of Numerical Analysis `doi.org/10.1093/imanum/dry029`.

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[12] B. Peherstorfer, K. Willcox, and M. Gunzburger; *Survey of multifidelity methods in uncertainty propagation, inference, and optimization*; SIAM Review **60** 2018, 550-591.

[13] D. Witman, M. Gunzburger, and J. Peterson; *Reduced-order modeling for nonlocal diffusion problems*; International Journal for Numerical Methods in Fluids **83** 2016, 307-327.

[14] H. Yang and M. Gunzburger; *Algorithms and analyses for stochastic optimization for turbofan noise reduction using parallel reduced-order modeling*; Computer Methods in Applied Mechanics and Engineering **319** 2017, 217-239.