Final Report
DOE-CSU-26128-1

DOE award number: DE-SC0009279
Institution: Colorado State University
Project title: DiaMonD: An Integrated Multifaceted Approach to Mathematics at the Interfaces of Data, Models, and Decisions
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Investigator: Troy Butler
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1. Center description and goals

For many problems in computational science and engineering, the so-called *forward* problem—solution of the underlying mathematical model to yield output quantities of interest, given input parameters—is difficult enough for frontier complex models, which are often characterized by coupled multiphysics and possibly stochastic behavior over a wide range of length and time scales. However, we face the need to move beyond the forward problem, to address what is often the ultimate goal of CS&E: *decision-making*. This requires us to tackle a spectrum of mathematical problems that subsume, and are thus even more difficult than, the forward problem. First, given experimental data, we wish to estimate unknown parameters characterizing a model of a natural or engineered system by solving an *inverse* problem. Second, we seek the optimal configuration of the system (or experiments) by solving an *optimal design* problem. Third, the optimal operation of the system must be determined by solving an *optimal control* problem. And fourth, we must *quantify uncertainties* as they propagate through all of the preceding problems, from data to model inference to prediction and finally to optimal design and control.

Optimal mathematical methods and algorithms for such *end-to-end, data-to-decisions modeling and simulation* of complex problems—requiring integrated solution of forward, inverse, optimization, and UQ problems for large, multiphysics, multiscale models—entails challenges of the highest order, while also presenting great opportunities for applied mathematics research. Unfortunately, research on forward, inverse, optimization, and UQ problems has all-too-often progressed in isolation. This has led to mathematical methods that perform well when considering the forward simulation in isolation, but are prohibitive or suboptimal or unstable when combined with other methods within the framework of inversion, optimization, or UQ. The reverse is also true: general-purpose methods developed within the inversion, optimization, and UQ fields often become prohibitive when applied to complex CS&E problems since they do not exploit their structure.

DiaMonD is a multi-institutional DOE MMICC effort that aims to address the challenges of end-to-end, data-to-decisions modeling and simulation for complex CS&E problems in a *unified, systematic, and integrated fashion*. Institutions involved are Colorado State, Florida State, Los Alamos, MIT, Oak Ridge, Stanford, and UT-Austin. The goals of DiaMonD are (1) to develop advanced mathematical methods and analysis for multimodel, multiphysics, multiscale model problems driven by frontier DOE applications, including those in subsurface energy and environmental flows, materials for energy storage and conversion, and ice sheet dynamics; (2) to create theory and algorithms for integrated inversion, optimization, and uncertainty quantification for these complex problems; and (3) to disseminate the philosophy of an integrated end-to-end, data-to-decisions approach to modeling and simulation of complex problems to the broader applied math and computational science communities through workshops and other outreach.

2. Personnel

2.1. Personnel directly supported by the CSU contract

- Don Estep, PI
- Troy Butler, project investigator, professor at University of Colorado Denver, working on stochastic inverse problems for differential equations
- Nishant Panda, postdoc at CSU and UCD, working on effects of model resolution and fidelity on stochastic inverse problems. Panda is now a postdoc at Los Alamos National Laboratory.
- Lei Yang, graduate student at CSU, working on stochastic inverse problems for differential equations. Lei earned a PhD and took a postdoc position at SAMSI.
- Yiming Yu, undergraduate student at CSU, working on stochastic inverse problems for differential equations. Yiming Yu graduated and went to graduate school.
- Michael Pilosov, graduate student at UCD, working on stochastic inverse problems. He will be defending his Phd thesis soon.
- Jiarui Chi is a Ph.D. student in Statistics at CSU who is still in progress.

2.2. Personnel supported in part by the CSU contract

- Jehanzeb Hameed Chaudhry, postdoc at Florida State University from postdoc at Colorado State University, working on a posteriori error analysis for reduced order modeling and use of ROM for a posteriori error estimation, jointly supervised by Max Gunzburger and Don Estep. Jehanzeb is now an assistant professor at University of New Mexico.

3. Overview of supported research

3.1. A posteriori error analysis for numerical methods used for coupled physics problems

The effort in this area focussed on two problems: (1) derive a posteriori error estimates for numerical solution of various coupled physics problems and (2) systematically develop a theory for a posteriori error estimation for numerical methods employing explicit methods, semi-explicit methods, or implicit methods with finite iteration for integration of time. The study of (2) is motivated by the fact that such techniques are prevalent in the numerical solution of multiphysics problems, but the ability to estimate their impact on accuracy has been lacking.

3.2. Stochastic inverse problems for differential equations

We investigated the formulation and solution of stochastic inverse problems based on measure-theoretic probability and differential geometry.

4. Professional Activities and Products

4.1. Publications

1. *A Measure-Theoretic Computational Method for Inverse Sensitivity Analysis III: Multiple Quantities of Interest*, T. Butler, D. Estep, S. Tavener, C. Dawson, and J.J. Westerink, SIAM/ASA Journal on Uncertainty Quantification, 2, 174-202 (2014)
2. *A posteriori error analysis for nite element methods with projection operators as applied to explicit time integration techniques*, J. Collins, D. Estep and S. Tavener, BIT, December 2014, DOI 10.1007/s10543-014-0534-9

3. *Uncertainty quantification for approximate p-quantiles for physical models with stochastic inputs*, D. Elfverson, D. Estep, F. Hellman, A. Malqvist, SIAM ASA J. Uncert. Quant., 2 (2014), 826-850
4. *A posteriori analysis for iterative solvers for non-autonomous evolution problems*, J. H. Chaudry, D. Estep, V. Ginting, and S. Tavener, SIAM ASA J. Uncert. Quant., 3 (2015), doi:10.1137/130949403
5. *A posteriori error analysis of IMEX time integration schemes for advection-diffusion-reaction equations*, J. Chaudry, D. Estep, V. Ginting, J. Shadid, and S. Tavener, CMAME, 285 (2014), 730-751
6. *A posteriori error estimates for mixed finite element and finite volume methods for parabolic problems coupled through a boundary with non-matching discretizations*, T. Arbogast, D. Estep, B. Sheehan, and S. Tavener, SIAM ASA J. Uncert. Quant., 3 (2015), 169-198
7. *Definition and solution of a stochastic inverse problem for the Manning's n parameter field in hydrodynamic models*, T. Butler, L. Graham, D. Estep, C. Dawson, and J.J. Westerink, Adv.Water Res., 78 (2015), 60–79
8. *Adaptive finite element solution of multiscale PDE-ODE systems*, A. Johansson, J. H. Chaudhry, V. Carey, D. Estep, V. Ginting, M. Larson, and S. Tavener, CMAME, 287 (2015), 150–171
9. *The interaction of iteration error and stability for linear partial differential equations coupled through an interface*, B. Sheehan, D. Estep, S. Tavener, J. Cary, S. Kruger, A. Hakim, A. Pletzer, J. Carlsson, and S. Vadlamani, Adv. Math. Physics, 2015, 13 pages, doi:10.1155/2015/787198
10. *Quantifying uncertainty in material damage from vibrational data*, T. Butler, A. Huhtala, and M. Juntunen, J. Comput. Physics, 283 (2015), 414-435
11. *On a perturbation method for stochastic parabolic PDE*, D. Estep and P. Polyakov, Comm. Math. Stat., 3 (2015), 215-226
12. *A posteriori error estimation for a cut cell finite volume method with uncertain interface location*, J. B. Collins, D. Estep, and S. Tavener, Intern. J. Uncert. Quant., 2015, to appear
13. *Parameter estimation and prediction for groundwater contamination based on measure theory*, Troy Butler, Clint Dawson, Donald Estep, Steven Mattis, Velimir Vesselinov, Water Res. Res., 52 (2015), 7808-7629
14. *A posteriori error analysis of two stage computation methods with application to efficient resource allocation and the Parareal Algorithm*, J. H. Chaudhry, D. Estep, S. Tavener, V. Carey, and J. Sandelin, SIAM Journal on Numerical Analysis, 54 (2016), 2729-3122
15. Exploration of efficient reduced-order modeling and a posteriori error estimation, J. H. Chaudhry, D. Estep, M. Gunzburger, International Journal on Numerical Methods for Engineering, 111 (2016), 102-122
16. *A stochastic inverse problem for multiscale models*, N. Panda, T. Butler, D. Estep, L. Graham, and C. Dawson, Journal for Multiscale Computational Engineering, 15 (2017), 265-283.
17. *A Measure-Theoretic Algorithm for Estimating Bottom Friction in a Coastal Inlet: Case Study of Bay St. Louis during Hurricane Gustav (2008)*, L. Graham, T. Butler, S. Walsh, C. Dawson, J.J. Westerink, Monthly Weather Review, 145, 929-954 (2017)
18. *Efficient distribution estimation and uncertainty quantification for elliptic problems on domains with stochastic boundaries*, J. H. Chaudhry, N. Burch, D. Estep, SIAM/ASA Journal on Uncertainty Quantification, 6 (2018), 1127-1150.
19. *Data-driven uncertainty quantification for predictive flow and transport modeling using support vector machines*, He, J., Mattis, S.A., Butler, T.D. et al. Comput Geosci (2018). https://doi.org/10.1007/s10596-018-9762-4
20. *Utilizing Adjoint-Based Error Estimates for Surrogate Models to Accurately Predict Probabilities of Events*, T. Butler and T. Wildey, International Journal for Uncertainty Quantification, 8(2): 143-159 (2018)

4.2. Software

Lindley Graham, Steven Mattis, Scott Walsh, Troy Butler, Michael Pilosov, and Damon McDougall (2016, August 10). BET: Butler, Estep, Tavener Method v2.0.0 (Version v2.0.0). Zenodo. http://doi.org/10.5281/zenodo.59964

4.3. Presentations

The PIs gave the following major presentations:

- D. Estep, Minitutorial on adjoint based a posteriori error estimation, Rocky Mountain Summer Workshop on Uncertainty Quantification, University of Colorado Denver, 7/15
- T. Butler, Quantifying Errors in a Probabilistic Solution to Stochastic Inverse Problems for Physics-Based Models, Minisymposium on Error Analysis and Scalability of UQ Methodologies for Inverse Problems at the SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 14-18, 2015
- T. Butler, BET: Algorithmic and Error Analyses, Minisymposterium on BET: Open Source Software for Stochastic Inverse Problems in a Measure-Theoretic Context, SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 14-18, 2015
- T. Butler, BET Tutorial and Demos, co-presenter, Rocky Mountain Summer Workshop on Uncertainty Quantification, Denver, CO, July 15-17, 2015
- T. Butler, Algorithms and error analysis of a measure theoretic framework for quantifying uncertainty, Rocky Mountain Summer Workshop on Uncertainty Quantification, Denver, CO, July 15-17, 2015
- T. Butler, Advances in High-Dimensional Computational Measure Theory for Inverse Problems, Minisymposium on Scalable Methods for Uncertainty Quantification at the 2015 US National Congress on Computational Mechanics Conference, San Diego, CA, July 26-30, 2015
- T. Butler, Non-Intrusive Algorithms for Measure-Theoretic Propagation of Uncertainties- Errors, Opportunities, and Challenges, Workshop on Numerical Methods for Large-Scale Nonlinear Problems and Their Applications, Institute for Computational and Experimental Research in Mathematics, Brown University, August 31 - September 4, 2015
- D. Estep, Fisk Distinguished Lecture, Department of Mathematics, University of Wyoming, 2015
- D. Estep, Research Collaboration Workshop: Optimization and Uncertainty Quantification in Energy and Industrial Applications, Institute for Mathematics and its Applications, University of Minnesota, Invited Talk, 2016
- D Estep, Short course on a new approach to stochastic inverse problems for scientific inference, Computational Mathematics, Department of Mathematical Sciences, Chalmers University of Technology, Gothenburg, Sweden, 2016
- D. Estep, Short Course on Duality, Adjoints, and A Posteriori Error Estimation, Wright Patterson Air Force Base, Dayton, Ohio, 2017
- D. Estep, Mathematics for Measurement, International Centre for Mathematical Sciences, Edinburgh, Scotland, Keynote Talk 6/17 27th Biennial Conference on Numerical Analysis, University of Strathclyde, Glasgow, Scotland, Plenary Talk, 2017
- D. Estep, SIAM Central States Section Meeting, Colorado State University, Fort Collins, Plenary Talk, 2017

The PIs gave many invited talks in addition to these.

4.4. Professional Activites and Distinctions

DOE-related Service

- D. Estep, Panel Chair, Beyond Interpretive Simulations, Fusion Energy Sciences and Advanced Scientific Computing Research Workshop on Integrated Simulations for Magnetic Fusion Sciences. Co-Author of Workshop Report. Department of Energy Office of Sciences, 2015.

Editorial Boards

- D. Estep, Editor in Chief (founding), SIAM/ASA Journal on Uncertainty Quantification, 2012 - 2017
- D. Estep, Editor in Chief, SIAM Book Series on Computational Science and Engineering, 2009 -
- D. Estep, Associate Editor, SIAM Journal on Numerical Analysis, 2005-
- D. Estep, Associate Editor, International Journal for Uncertainty Quantification, 2010 -
- D. Estep, Advisory Editor, International Journal of Computer Mathematics, 2012 -
- D. Estep, Associate Editor, Multiphysics Modeling Book Series, A. A. Balkema Publishing, 2009-
- D. Estep, Associate Editor, Journal of Applied Mathematics and Computing, 2008-

Professional Meeting Organization

- T. Butler, Minisymposium on Error Analysis and Scalability of UQ Methodologies for Inverse Problems, SIAM CSE 2015, Sale Lake City, UT
- T. Butler, Rocky Mountain Summer Workshop on Uncertainty Quantification, University of Colorado Denver, July 2015
- D. Estep, Workshop on Uncertainty Quantification, Mittag-Leffler Institute, Stockholm, Sweden, 2016
- D.Estep, Workshop on UQ for Inverse Problems in Complex Systems, Isaac Newton Institute, Cambridge, United Kingdom, Principal Organizer, 2018