Final Report

February 9, 2019

Title: Active Subspace Methods for Data-Intensive Inverse Problems
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Project description and goals

Inverse problems are pervasive in engineering and science, especially in scientific discovery and decision-making for complex, physical, and environmental systems. They are perhaps the most popular mathematical approaches for *enabling predictive scientific simulations* that *integrate observational data, experimental data, simulations and/or models.* For inverse problems that serve as a basis for design, control, discovery, and decision-making, the uncertainty in their solutions must be quantified. However, unless equipped with advanced mathematical algorithms, uncertainty quantification (UQ) in high dimensional parameter spaces would require exponential increase in computing effort, and this would be beyond current petascale and future exascale computing capabilities. Though the past decades have seen tremendous advances in both mathematical theories and computational algorithms for inverse problems, quantifying the uncertainty in their solution remains an open problem facing the computational science and engineering community. On the other hand, the exponential increase in the quantity of measurements and data holds tremendous promise for data-driven scientific discoveries. However, much data remains unused as inversion and UQ methods—a systematic tool to infer knowledge from data—are unable to scale up to the quantity of data being generated. *Thus, there is a critical need to develop scalable mathematical and computational algorithms to tackle the challenge of* large-scale UQ problems *in* high dimensional parameter space *with* big data *in order to harness the potential of extreme computing to enable predictive scientific simulations and to further science discoveries.*

The goal of this project is to develop advanced mathematical methods/algorithms to address the challenges associated with big-data and high dimensional parameter spaces for large-scale inverse/UQ problems.

significant findings and conclusions

There are many approaches to explore the Bayesian posterior distribution to estimate the mean and the associated uncertainty. We argue that Markov chain Monte Carlo (MCMC) methodology is a viable option to tackle large-scale complex problems. The problem is, however, that standard MCMC methods often require millions of samples, and hence millions of expensive forward simulations, to converge. This is mainly due to samples being strongly correlated with each other, consequently slowing down the mixing and hence the convergence. In extremely high dimensional parameter spaces, i.e. problems we are facing in this project, standard MCMC methods become infeasible.

We have proposed the adoption of a computationally inexpensive Riemann manifold Hamiltonian Monte method to explore the posterior of large-scale Bayesian inverse problems governed by PDEs in a highly efficient manner. We first adopt an infinite dimensional Bayesian framework to guarantee that the inverse formulation is well-defined. In particular, we postulate a Gaussian prior measure on the parameter space and assume regularity for the likelihood. This leads to a well-defined posterior distribution. Then, we discretize the posterior using the standard finite element method and a matrix transfer technique. Our result is a constructive and discretization-invariant FEM method for infinite dimensional MCMC methods. **T**his work has been published in Inverse Problems and Imaging [6].

We then apply the Riemannian Hamiltonian MCMC (RMHMC) approach on the resulting discretized posterior in finite dimensional parameter space. We present an adjoint technique to efficiently compute the gradient, the Hessian, and the third derivative of the potential function that are required in the RMHMC context. This is at the expense of solving a few extra PDEs: one for the gradient, two for a Hessianvector product, and four for the product of third order derivative with a matrix. For large-scale problems, repeatedly computing the action of the Hessian and third order derivative is too computationally expensive and this motivates us to design a simplified RMHMC in which the Fisher information matrix is computed once at the MAP point. We further reduce the effort by constructing low rank approximation of the Fisher information using a randomized singular value decomposition technique. The beauty of this method is that its acceptance rate is almost unity (the best possible). We have also shown that though data is intensive, they are not independent. In particular, data typically inform a subspace with reasonably small dimension compared to that of the unknown solution. *We explore this fact to construct this active subspace from a low rank approximation of the Hessian for our Riemannian Hamiltonian MCMC.* The effectiveness of the proposed approach is demonstrated on a number of numerical results up to 1025 parameters in which the computational gain is about two orders of magnitude while maintaining the quality of the original RMHMC method in generating (almost) uncorrelated/independent samples. **T**his work has been published in Inverse Problems [5].

To accelerate our RMHMC method, we have developed Gaussian process approximation to approximate the gradient, the Hessian, and the third derivative tensor. This allows us to compromise the effectiveness of RMHMC exploration of the parameter space and the low cost of Gaussian process. We have demonstrated our methods on subsurface flow, a DOE relevant application, and compared our method against standard RMHMC and a variety of other methods. We have seen that our method is orders of magnitude more efficient in exploring high dimensional parameter spaces while having comparably low computational cost. **T**his work has been publish in the Journal of Computational Physics [8].

The PI, together with Paul Constantine (CSM PI), have collaboratively developed an active subspace method in which we first reduce the dimension of the parameter space and then perform MCMC on the reduced subspace. This allows us to use straightforward standard MCMC methods while efficiently exploring the posterior in high dimensional parameter spaces with a fraction of the cost. Our idea is to seek the low dimensional active reduced subspaces that is informed by the data. Since the data is limited, it encodes limited information. We have established the mathematical proof for this fact from our previous work on the compactness of the misfit Hessian. This provides a solid foundation for our active subspace methods. Once the active reduced subspace is found, we perform standard MCMC on this low dimensional active subspace and draw exact independent samples for other inactive parameters using the prior distribution. We have successfully demonstrated the scalability and effectiveness of our approach for both analytical example and practical setting for inverse elliptic problems in two spatial dimensions. **T**his work has been published in the SIAM Journal on Scientific Computing [7].

The exponential increase in the quantity of measurements and data holds tremendous promise for data-driven scientific discovery. However, much of data remains unused as inversion methods—a systematic tool to infer knowledge from data—are unable to scale up to the amount of data. One of the main reasons is that the level of informativeness of the data is measured, roughly speaking, in terms of the number of independent data with which the number of simulations scales. Indeed, in general, the more the number of independent data is, the higher the rank of the Hessian, and hence the more the number of forward solves. This makes contemporary Newton-like and structure-exploiting inversion methods in which the Hessian is the key player, impractical. Moreover, the imbalance between the amount of data that we can fit in memory, and what we wish to process is only going to increase in the foreseeable future. While significant research has been done on various aspects of large-scale inverse problems, little work has been done on developing algorithms that are both computationally as well as data scalable. *We now present our ideas that we have explored to address this challenge.*

We have developed a randomized misfit approach (RMA) for **e**fficient data reduction in large-scale inverse problems. The method is a random transformation approach that generates **a**ctive data subspace by randomly combining the original ones. Our main idea is to first randomize the misfit and then use the sample average approximation to solve the resulting stochastic optimization problem. At the heart of our approach is the blending of the stochastic programming and the random projection theories, which brings together the advances from both sides and exploits opportunities at their interfaces. This allows us to conduct a more complete analysis of the RMA method, which is unlikely possible using sole theory from either of the communities separately. One of the main results of the paper is the interplay between the Johnson-Lindenstrauss lemma and large deviation theory. In particular, the former provides sharp bounds on the **a**ctive data dimensions for a large class of interesting sparse random transformations, while the latter introduces a new look and proof of the former. To justify the RMA approach, a detailed theoretical analysis is carried out for both linear and nonlinear inverse problems. A tight connection between the Morozov discrepancy principle and the Johnson-Lindenstrauss lemma is presented. It is this connection that allows us to explain the ability of the RMA method in significantly reducing observation data with quantifiable accuracy lost for the solution of inverse problems. Various numerical results to motivate and to verify our theoretical findings are presented for inverse problems governed by elliptic partial differential equations in one, two, and three dimensions. We, the PI and *two graduate students hired to work on this project*, **h**ave completed a paper on this method have published it in Inverse Problems [9]. Besides this, we have also published two papers on the subjects but with different methods [12, 1].

We have also developed efficient numerical discretization for the forward equation to reduce the cost of the forward solve while exploiting current and future computing system with massive parallelism. This will help speed up solution of inverse problems governed by partial differential equations (PDEs). In particular, we have developed a unified hybridized discontinuous Galerkin (HDG) framework that can constructively derive HDG methods for a wide range of PDEs relevant to DOE including elliptic, parabolic, hyperbolic, and mixed type equations. HDG is an implicit high order discontinuous Galerkin method with the unique property that the coupled unknowns reside on the mesh skeleton, i.e. the faces, and hence are substantially less compared to DG or spectral element methods. Furthermore, once the traces are solved for, volume unknowns can be recovered element-by-element completely in parallel. It is therefore well suited for projected highly multi-threaded exascale supercomputer technologies. We have successfully developed HDG methods for PDEs arising in climate prediction including shallow water equations and stratified Euler equations on spheres. **W**e have published five papers on this development [2, 3, 4, 10, 11].

What we have accomplished is more than what we promised in the original proposal. In fact, we have finished not only planned items in the proposal but also those which were not in the proposal but directly support overarching theme of the proposal.

Funded students

The PI has used this award and other awards to support four graduate students during the project time: Ellen Le, Aaron Myers, and Stephen Shanoon, all are ICES students, and Shinhoo Kang, an aerospace engineering student.

Publications, presentations, and organization

Publications [13]

1. **Bui-Thanh**, T., and Ghattas, O., "A Scalable MAP Solver for Bayesian Inverse Problems with Besov Priors", *Inverse Problems and Imaging*, 9(1), pp. 27–53, 2015.

2. **Bui-Thanh**, T., "From Rankine-Hugoniot Condition to a Constructive Derivation of HDG Methods" *in Lecture Notes in Computational Science and Engineering*, 2015.

3. **Bui-Thanh**, T., "From Godunov to A Unified Hybridized Discontinuous Galerkin Framework" *Journal of Computational Physics*, 295, pp. 114-146, 2015.

4. Wilcox, L., Stadler, G., **Bui-Thanh**, T., and Ghattas, O., "Discretely exact derivatives for hyperbolic PDE-constrained optimization problems discretized by the discontinuous Galerkin method" *Journal of Scientific Computing*, 63, pp. 138–162, 2015.

5. Wang, K., T, **Bui-Thanh**, and Ghattas, O. "An rMAP Method for Nonlinear Bayesian Inverse Problems" SIAM Journal on Scientific Computing, 40(1), pp. A142–A171, 2018.

6. Constantine, P., Kent, C., **Bui-Thanh**, T. "Accelerating MCMC with Active Subspaces", SIAM Journal on Scientific Computing, 38(5), pp. A2779–A2805 , 2016.

7. Lan, S., **Bui-Thanh**, T., Christie, M., and Girolami, M., "Emulation of higher-order tensors in manifold Monte Carlo methods for Bayesian Inverse Problems", Journal of Computational Physics , 308, 81–101, 2016.

8. Le, E., Myers, A., and **Bui-Thanh**, T., "A Randomized Misfit Approach for Data Reduction in Large-Scale Inverse Problems", Inverse Problems, 33(6), 065003, 2017.

9. **Bui-Thanh**, T., " FEM-Based Discretization-Invariant MCMC Methods for PDE-constrained Bayesian Inverse Problems", Inverse Problems and Imaging, 10(4), pp. 943–975, 2016.

10. **Bui-Thanh**, T., "Hybridized Discontinuous Galerkin Methods for Linearized Shallow Water Equations", SIAM Journal on Scientific Computing, 38(6),pp. A3696–A3719, 2016.

11. Muralikrishnan, S., Tran, M-B, and **Bui-Thanh**, T., "iHDG: an iterative HDG Framework for Partial Differential Equations", SIAM Journal on Scientific Computing , 39(5), pp. S782–S808, 2017.

12. Muralikrishnan, S., Tran, M.B., and **Bui-Thanh**, T., "An improved iterative HDG approach for partial differential equations", Journal of Computational Physics, 367, pp. 295-321, 2018.

13. Alger, N., Villa, U., **Bui-Thanh**, T., and Ghattas, O., "A Data Scalable Augmented Lagrangian KKT Preconditioner for Large-scale Inverse Problems", SIAM Journal on Scientific Computing , 39(5), pp. A2365-A2393, 2017.

Invited presentations [34]

1. "Ensemble-based MCMC methods for exploring large-scale high dimensional Bayesian inverse problems", 8th International Congress on Industrial and Applied Mathematics, August, Beijing, China
2. "A randomized likelihood method for data reduction in large-scale inverse problems", 8th International Congress on Industrial and Applied Mathematics, August, Beijing, China
3. "An Approach to Big-Data in Large-Scale PDE-Constrained Bayesian Inverse Problems in High-Dimensional Parameter Spaces", 13th US National Congress on Computational Mechanics, San Diego, 2015
4. "A Large-Scale Ensemble Transform Method for Bayesian Inverse Problems Governed by PDEs", 13th US National Congress on Computational Mechanics, San Diego, 2015
5. "DG for Large-Scale Inverse Problems in Time Domain: Opportunities and Challenges", SIAM Conference on Mathematical and Computational Issues in Geosciences, Stanford, CA, 2015.
6. "A hybridized discontinuous Galerkin method for earth system models' dynamical cores", Galerkin methods with applications in weather and climate forecasting, Scotland, 2015
7. "Some Recent Advances in Hybridized Discontinuous Galerkin Methods", 1st Pan-American Congress on Computational Mechanics, Buenos Aires, 2015.
8. "Ensemble Methods for Large-Scale PDE-Constrained Bayesian Inverse Problems", SIAM Conference on Computational Science and Engineering, Utah, 2015.
9. "Some Recent Advances in Hybridized Discontinuous Galerkin Methods", Workshop on advanced Numerical Methods in the Mathematical Sciences, Texas A&M, 2015.
10. "Recent advances in solution of large-scale Bayesian inverse problems", Finland, Applied Inverse Problem Conference, 2015.
11. "A hybridized discontinuous Galerkin method for earth system models' dynamical cores", Galerkin methods with applications in weather and climate forecasting, Scotland, 2015
12. "DG for Large-Scale Inverse Problems in Time Domain: Opportunities and Challenges", SIAM Conference on Mathematical and Computational Issues in Geosciences, Stanford, CA, 2015. (Invited)
13. "A Large-Scale Ensemble Transform Method for Bayesian Inverse Problems Governed by PDEs", 13th US National Congress on Computational Mechanics, San Diego, 2015 (Invited)
14. "An Approach to Big-Data in Large-Scale PDE-Constrained Bayesian Inverse Problems in High-Dimensional Parameter Spaces", 13th US National Congress on Computational Mechanics, San Diego, 2015 (Invited)
15. "Towards Large-scale Computational Engineering and Sciences with Quantifiable Uncertainty", John Von Neumann Institute, Vietnam National Universities, 2015. (Invited)
16. "A randomized likelihood method for data reduction in large-scale inverse problems", 8th International Congress on Industrial and Applied Mathematics, August, 2015, Beijing, China (Invited)
17. "Ensemble-based MCMC methods for exploring large-scale high dimensional Bayesian inverse problems", 8th International Congress on Industrial and Applied Mathematics, August, Beijing, China (Invited)

18. “A Randomized likelihood approach for data reduction in large-scale inverse problems”, Texas Consortium for Computational Seismology, UT Austin, Fall 2015. (Invited)

19. “An Updated on Hybridized Discontinuous Galerkin Method for Non-Hydrostatic Atmosphere”, PDE on Spheres, Korea, October, 2015.

20. “Towards Large-scale Computational Engineering and Sciences with Quantifiable Uncertainty”, Petroleum and Geosystems Engineering Department, UT Austin, Spring 2016. (Invited)

21. “Particle-based Approximate Monte Carlo approaches for Large-Scale Bayesian Inverse Problems”, 12th International Conference on Monte Carlo and Quasi-Monte Carlo methods in Scientific Computing, Stanford, August, 2016. (Invited)

22. “Towards Large-scale Computational Engineering and Sciences with Quantifiable Uncertainty”, Sandia National Lab, New Mexico, August, 2016. (Invited)

23. “A Partial Domain Inversion Approach for Large-scale Baysian Inverse Problems in High Dimensional Parameter Spaces”, SIAM UQ conference, Lausanne, April, 2016. (Invited)

24. “A Randomized likelihood approach for data reduction in large-scale inverse problems”, SIAM UQ conference, Lausanne, April, 2016. (Invited)

25. “A Triple Model Reduction for Data-Driven Large-Scale Inverse Problems in High Dimensional Parameter Spaces”, SIAM UQ conference, Lausanne, April, 2016. (Invited)

26. “A fresh look at the Bayesian theorem from information theory”, ICES-Babuska series, seminar, Austin, September, 2016 (invited)

27. “A Randomized Misfit Approach for Data-Driven PDE-constrained Bayesian Inverse Problems”, Workshop on Uncertainty quantification and data-driven modeling, Austin, March 2017 (invited)

28. “Towards Large-Scale Computational Science and Engineering with Quantifiable Uncertainty”, Mini Workshop on Bayesian Inverse Problems and Imaging, May, 2017 (invited)

29. “The upwind hybridized discontinuous Galerkin (HDG) framework: Theory and application to magnetohydrodynamic and atmospheric applications”, Ninth Meeting on Numerical Analysis of Partial Differential Equations, Santiago, Chile, June 2017 (invited)

30. “The upwind hybridized discontinuous Galerkin (HDG) framework: Theory and application to magnetohydrodynamic and atmospheric applications”, VII International Congress on numerical methods, Guadalajara, Mexico, June, 2017 (Invited)

31. “Towards Large-Scale Computational Science and Engineering with Quantifiable Uncertainty”, workshop on Uncertainty Quantification, Guanajuato, Mexico, January, 2017 (Invited)

32. “Some advances in the upwind hybridized discontinuous Galerkin method for dynamical cores”, PDE on Spheres, France, April, 2017

33. “Model Reduction via Domain Truncation for Efficient Monte-Carlo Simulations of Large-Scale Bayesian Inverse Problems”, SIAM Conference on Computational Science and Engineering, Atlanta, March, 2017 (Invited)

34. “A data-scalable randomized misfit approach for solving large-scale PDE-constrained inverse problems”, Vietnam University of Science, Ha Noi, Vietnam, May, 2017 (Invited)

35. "A data-scalable randomized misfit approach for solving large-scale PDE-constrained inverse problems", John von Neumann Institute, Ho Chi Minh City, Vietnam, June, 2017 (Invited)

36. "A data-scalable randomized misfit approach for solving large-scale PDE-constrained inverse problems", SIAM conference on mathematical and computational issues in the Geosciences, Erlangen, Germany, September, 2017 (Invited)

37. "The upwind Hybridized discontinuous Galerkin method for dynamical cores", Mathematics of the Weather, Erquy, France, October, 2017 (Invited)

Lectures at international schools [10]

1. Invited Lecturer at the international winter School on UQ, Norway, January 2015

2. Invited Lecturer at EU Regional School, Course 7, UQ, Aachen, Germany, 2015

3. Invited lecturer at Texas Consortium for Computational Seismology, April, 2016

4. Invited speaker at the workshop on Uncertainty Quantification, Guanajuato, Mexico, January, 2017

5. Plenary speaker at the Ninth Meeting on Numerical Analysis of Partial Differential Equations, Santiago, Chile, June 2017

6. Plenary speaker at the VII International Congress on numerical methods, Guadalajara, Mexico, June, 2017

7. Invited speaker at the workshop on Uncertainty Quantification and Data-Driven Modeling, Austin, March, 2017

8. Invited speaker at the mini Workshop on Bayesian Inverse Problems and Imaging, Shanghai, May, 2017

9. Plenary speaker at MATHEMATICS FOR ATMOSPHERIC-BIOSPHERIC SCIENCE conference, Levi, Finland, November, 2017

10. Invited speaker at the workshop on Sensor location in Distribution parameter systems, Institute for Mathematics and its Applications, Minnesota, September, 2017

Organization [13]

1. Organizer of the Minisymposium on "Recent Advances in High Order Discontinuous Galerkin Methods" ICOSAHOM 14, Salt Lake City, Utah, 2014.

2. Organizer of the Minisymposium on "Uncertainty Modeling and High Performance Stochastic Methods for Computationally Intensive Calibrations, Predictions and Optimizations" WCCM 14, Barcelona, Spain, 2014

3. Organizer of the minisymposium on "Theory Implementation and Applications of HDG Methods" at the SIAM Conference on Computational Science and Engineering, Utah, 2015

4. Organizer of the minisymposium on "Recent Advances in High Order Finite Element Methods for Atmospheric Sciences" at the SIAM Conference on Computational Science and Engineering, Utah, 2015

5. Organizer of the minisymposium on "Higher Order Finite Element Discretizations" at the 1st Pan- American Congress on Computational Mechanics, Buenos Aires, 2015

6. Organizer of the minisymposium on "Recent Advances in Higher Order Finite Element Methods" at the 13th US National Congress on Computational Mechanics, San Diego, 2015
7. Organizer of the minisymposium "Advances in MCMC and related sampling methods for large-scale inverse" at the 8th International Congress on Industrial and Applied Mathematics, August, 2015, Beijing, China
8. Organizer of the minisymposium "Inverse Problems meet big data", at the SIAM Conference on Uncertainty Quantification, Lausanne, April, 2016.
9. Organizer of the minisymposium "Advances in Sampling Methods for Bayesian Inverse Problems", at the SIAM Conference on Uncertainty Quantification, Lausanne, April, 2016.
10. Organizer of the minisymposium "Advances in Sampling Methods for Bayesian Inverse Problems", at the SIAM Conference on Uncertainty Quantification, Lausanne, April, 2016.
11. Organizer of the minisymposium "Inverse Problems meet big data", at the SIAM Conference on Computational Science and Engineering, Atlanta, 2017
12. Organizer of the minisymposium "Efficient Algorithms for Bayesian Inverse Problems Governed by PDE Forward Problems", at the SIAM Conference on Computational Science and Engineering, Atlanta, 2017
13. Organizer of the minisymposium "Advances in MCMC and Related Sampling Methods for Large-Scale Inverse Problems", at the SIAM Conference on Computational Science and Engineering, Atlanta, 2017 Organizer of the minisymposium "Advances Approaches for PDE-Constrained Bayesian Inverse", at the SIAM Annual Meeting, Atlanta, July, 2017

References

[1] N. Alger, U. Villa, T. Bui-Thanh, and O. Ghattas, *A data scalable augmented Lagrangian KKT preconditioner for large-scale inverse problems*, SIAM Journal on Scientific Computing, 39 (2017), pp. A2365–A2393. http://users.ices.utexas.edu/%7Etanbui/PublishedPapers/dataScalableInverse.pdf.

[2] T. Bui-Thanh, *From godunov to a unified hybridized discontinuous Galerkin framework for partial differential equations*, Journal of Computational Physics, 295 (2015), pp. 114–146. http://users.ices.utexas.edu/%7Etanbui/PublishedPapers/unifiedHDG.pdf.

[3] T. Bui-Thanh, *From Godunov to a unified hybridized discontinuous Galerkin framework for partial differential equations*, Journal of Computational Physics, 295 (2015), pp. 114–146. http://users.ices.utexas.edu/%7Etanbui/PublishedPapers/unifiedHDG.pdf.

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[5] T. Bui-Thanh and M. A. Girolami, *Solving large-scale PDE-constrained Bayesian inverse problems with Riemann manifold Hamiltonian Monte Carlo*, Inverse Problems, Special Issue (2014), p. 114014. http://users.ices.utexas.edu/%7Etanbui/PublishedPapers/RMHMC.pdf.

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[8] S. Lan, T. Bui-Thanh, M. Christie, and M. Girolami, *Emulation of higher-order tensors in manifold monte carlo methods for bayesian inverse problems*, Journal of Computational Physics, 308 (2016), pp. 81 – 101.

[9] E. B. Le, A. Myers, T. Bui-Thanh, and Q. P. Nguyen, *A data-scalable randomized misfit approach for solving large-scale pde-constrained inverse problems*, Inverse Problems, 33 (2017), p. 065003. https://arxiv.org/pdf/1603.01562.pdf.

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[12] K. Wang, T. Bui-Thanh, and O. Ghattas, *A Randomized Maximum A Posteriori Method for Posterior Sampling of High Dimensional Nonlinear Bayesian Inverse Problems*, SIAM Journal of Scientific Computing, Accepted, (2018). https://arxiv.org/pdf/1602.03658.pdf.