Final Report: Large-Scale Optimization for Bayesian Inference in Complex Systems

Project duration: Aug. 15, 2008 – Aug. 14, 2012 (2013 for MIT)

Joint report submitted by Massachusetts Institute of Technology (DE-FG02-08ER25858), University of Texas at Austin (DE-FG02-08ER25860), Georgia Institute of Technology

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1 Summary

The SAGUARO (Scalable Algorithms for Groundwater Uncertainty Analysis and Robust Optimization) Project focuses on the development of scalable numerical algorithms for large-scale Bayesian inversion in complex systems that capitalize on advances in large-scale simulation-based optimization and inversion methods. Our research is directed in three complementary areas: efficient approximations of the Hessian operator, reductions in complexity of forward simulations via stochastic spectral approximations and model reduction, and employing large-scale optimization concepts to accelerate sampling. Our efforts are integrated in the context of a challenging testbed problem that considers subsurface reacting flow and transport.

The MIT component of the SAGUARO Project addresses the intractability of conventional sampling methods for large-scale statistical inverse problems by devising reduced-order models that are faithful to the full-order model over a wide range of parameter values; sampling then employs the reduced model rather than the full model, resulting in very large computational savings. Results indicate little effect on the computed posterior distribution. On the other hand, in the Texas–Georgia Tech component of the project, we retain the full-order model, but exploit inverse problem structure (adjoint-based gradients and partial Hessian information of the parameter-to-observation map) to implicitly extract lower dimensional information on the posterior distribution; this greatly speeds up sampling methods, so that fewer sampling points are needed. We can think of these two approaches as “reduce then sample” and “sample then reduce.” In fact, these two approaches are complementary, and can be used in conjunction with each other. Moreover, they both exploit deterministic inverse problem structure, in the form of adjoint-based gradient and Hessian information of the underlying parameter-to-observation map, to achieve their speedups.

Reduced-order models for large-scale statistical inverse problems. One MIT component of the SAGUARO Project focuses on the role of reduced-order models to accelerate conventional sampling methods for large-scale statistical inverse problems. Our research developed new methodology for performing model reduction in both parameter and state spaces. This permits sampling (using a method such as Markov chain Monte Carlo (MCMC)) to be carried out in a low-dimensional reduced parameter space, and also accelerates the many forward model evaluations required to sample the posterior. The challenge of determining reduced-order models in this setting is to come up with a basis that effectively spans the parameter space of interest, an especially difficult task when the parameter space is of high dimension. We address this challenge by formulating the model reduction task as an optimization problem, which we solve using a heuristic but efficient greedy approach that exploits adjoint-based gradients and Hessian information of the parameter-to-observation map.

Inference for prediction. Another component of the MIT effort is the development of a

goal-oriented approach to inference of large-scale systems. Inference of model parameters is often one step in a process ending in predictions that support decision in the form of design or control. Incorporation of end goals into the inference process leads to more efficient goal-oriented algorithms that automatically target the most relevant parameters for prediction. In the linear setting, our approach to goal-oriented inference exploits a compelling connection to balanced truncation model reduction. In balanced truncation one obtains a projection-based reduced model that balances the controllability and observability of the underlying transformed system. In the goal-oriented inference context, we present an approach that leads to a balance between the experiment and prediction observability associated with parameter modes. In the linear case, this approach leads to a form of subspace regularization that is dimensionally optimal in the sense that we infer the fewest number of parameters necessary to accurately estimate the predictions required to meet end goals. The inference-for-prediction method exactly replicates the prediction results of either truncated singular value decomposition, Tikhonov-regularized, or Gaussian statistical inverse problem formulations independent of data; it sacrifices accuracy in parameter estimate for online efficiency.

Stochastic spectral methods for statistical inverse problems. Another MIT effort focuses on stochastic spectral methods, which exploit regularity in the dependence of the forward model—both its internal state and outputs—on uncertain parameters. These methods can be applied intrusively (e.g., in a Galerkin formulation) or non-intrusively (e.g., via collocation); the former requires a reformulation of the governing equations, while the latter requires only deterministic forward simulations at a sparse set of quadrature points. In either case, using stochastic spectral methods to propagate prior uncertainty through the forward model yields a surrogate posterior density that is extremely inexpensive to evaluate, often orders of magnitude faster than the true posterior. We established new convergence results that tie the L^2 convergence rate of a stochastic spectral forward solution to the convergence rate, in Kullback-Leibler divergence, of the surrogate posterior distribution. These results were demonstrated numerically on problems with smooth and with discontinuous dependence on the inversion parameters, and with unimodal or multi-modal posterior distributions. Additional computational work focused on the inversion of spatially distributed parameters in a prototypical porous media problem; here, dimensionality reduction was achieved through Karhunen-Loève representations of Gaussian process priors. The inverse problem was cast in a hierarchical Bayesian formulation, where we inferred not only the permeability field but regularization parameters—or equivalently, prior hyperparameters—from data. Ongoing work targets scalability of the stochastic spectral approach to even higher-dimensional inverse problems, where we will improve upon the Karhunen-Loève basis by combining prior information with low-rank approximations of the Hessian.

We have also carried out a detailed comparison between non-intrusive stochastic spectral approximations and projection-based reduced models, articulating the relative advantages and disadvantages of each method in the context of a representative source inversion problem. We show that if the number of full model samples available to create the approximate models is small, then the projection-based approach achieves a more accurate solution to the inverse problem. If however a sufficient number of samples can be used for stochastic collocation, the resulting models are several times more efficient to solve than a reduced-order model of comparable accuracy.

Exploiting PDE problem structure in large-scale statistical inverse problems. The Texas-Georgia Tech component of the SAGUARO Project is aimed at creating MCMC methods that are enhanced with knowledge of problem structure. Unlike conventional MCMC methods that view the mapping between the uncertain parameters and the observations as a black box, here we capitalize on structural information commonly exploited in deterministic PDE-based inverse problems, in particular the gradient and Hessian of the parameter-to-observation map (computed using adjoint-based approaches). Our work is based on Langevin dynamics, which we interpret as

a “stochastic steepest descent” for the posterior. Based on this interpretation, we have extended the Langevin idea to include preconditioning by the inverse of the Hessian, rendering a “stochastic Newton” method. The Langevin step is taken as a proposal for an MCMC method. Effectively, our stochastic Newton MCMC method builds a local Gaussian approximation of the posterior pdf based on local gradient and Hessian information (of the negative log posterior), and then draws a sample from it as a proposal for Metropolis-hastings MCMC. This is analogous to the classical Newton method’s construction of a local quadratic approximation of a function (based on gradient and Hessian information), which is then minimized to compute the next point in the iterative process. We were able to prove that in the limit of a Gaussian posterior, our stochastic Newton MCMC method exactly samples the posterior, so that each sample is accepted with probability 1. The central advantage of this method is that it tailors the proposal to the shape (as defined by the Hessian) of the posterior pdf; this is important for ill-posed inverse problem, which tend to have highly stretched contours, resulting from some directions in parameter space being well-informed by the data, and others being poorly informed (or not informed at all).

A critical aspect of the stochastic Newton method is the need to manipulate the Hessian matrix, and in particular to compute the square root of its inverse. Ordinarily, this would be an intractable task, since merely computing the Hessian (let alone factoring it) requires n forward PDE solves, where n is the dimension of the (discretized) parameter field. Moreover, the Hessian would have to be constructed at each MCMC iteration! The key new idea was to recognize that for many ill-posed inverse problems (including the target subsurface flow inverse problem), the Hessian is a compact operator with rapidly-decaying eigenvalues, and thus it can be efficiently represented by a low-rank approximation consisting of the dominant eigenpairs. The dominant eigenpairs can be extracted efficiently through a Lanczos method, or else through a randomized SVD. The result is a Hessian approximation that can capture the behavior of the full Hessian to any desired degree of accuracy, while requiring typically a small number of forward PDE solves, independent of problem size (compression rates can be as low as 0.1%). The intuition behind the low-rank approximation is that the data typically contain finite-dimensional information and are informative about a low-dimensional subspace of the infinite dimensional field we seek to reconstruct in the inverse problem. We have proven the compactness of the Hessian for several problems, including a model subsurface flow problem.

We have applied our low-rank, Hessian-accelerated MCMC ideas to several problems including those in subsurface flow, and have several orders of magnitude speedups over reference MCMC methods for modest problems. For were able to solve several large-scale Bayesian inverse problems with thousands to hundreds of thousands of parameters, for which conventional methods were unable to solve.

Representer-based schemes for data inversion. Another research activity at The University of Texas (collaborative between C. Dawson and M. Iglesias at MIT) is the investigation of parameter estimation techniques based on data assimilation methods, particularly the so-called representer method. This method has been investigated for data assimilation problems in the fields of meteorology, oceanography and petroleum engineering. Iglesias and Dawson have previously investigated this approach for the estimation of hydraulic conductivity in single phase ground water flow. For linear data assimilation problems, the representer method gives an exact solution to the Euler-Lagrange equations arising from minimizing the cost functional representing the misfit between measurements and model. For parameter estimation, the model becomes nonlinear (even for linear forward models), therefore Iglesias and Dawson have proposed an iterative representer-based method where the nonlinear model is linearized around prior information (forward model solution and prior hydraulic conductivity), and the Euler-Lagrange equations arising from this linearized model are solved using the Representer Method. Convergence results have been proved for this

approach, assuming certain smoothness on the forward model and that the prior parameter model is sufficiently close to the true parameter. We have also investigated the use of Karhunen-Loève expansions of hydraulic conductivity, which preserve geological consistency (important when certain geostatistics are known about conductivity), and reduce the parameter estimation problem from field estimation to the estimation of a few coefficients in the K-L expansion (greatly reducing computational expense). Current work is focused on extending these approaches to multiphase flow in the subsurface and to ground water flow coupled with contaminant transport.

2 Personnel Supported

MIT: 1 graduate student, 1 postdoc

UT Austin: 1 graduate student, 0.5 postdoc

Georgia Tech/UT Austin: 1 postdoc (PI Biros moved to UT Austin in 2011)

Sandia/MIT: 1 technical staff (Aug.-Dec. 2008), 1 postdoc (PI Marzouk moved to MIT in 2009)

3 Publications, Talks, Awards

Publications

1. S.S. Adavani and G. Biros, Multigrid solvers for inverse problems with parabolic PDE constraints, *SIAM Journal on Scientific Computing*, Vol. 31, No. 1, pp. 369–397, 2008.
2. G. Biros and G. Doğan, A multilevel algorithm for inverse problems with elliptic PDE constraints, *Inverse Problems*, Vol. 24, No. 3, pp. 1–19, 2008.
3. M. Iglesias and C. Dawson, An iterative representer-based scheme for data inversion in reservoir modeling, *Inverse Problems*, 25, 34 pp., 2009.
4. S.S. Adavani and G. Biros, Fast algorithms for source identification problems with elliptic PDE constraints, *SIAM Journal on Imaging Sciences*, 3 (4), pp. 791–808, 2010.
5. G. Biros and G. Doğan, A fast inversion algorithm for linearized diffuse optical tomography with many measurements, submitted for publication.
6. C. Burstedde and O. Ghattas, Algorithmic strategies for full waveform inversion: 1D experiments, *Geophysics*, 74(6):WCC37WCC46, 2009.
7. J. Martin, L.C. Wilcox, C. Burstedde, and O. Ghattas, A Stochastic Newton MCMC method for large-scale statistical inverse problems with application to seismic inversion, *SIAM Journal on Scientific Computing*, 34(3):A1460-A1487, 2012.
8. M Iglesias, C Dawson, “An iterative representer-based scheme for data inversion in reservoir modeling,” *Inverse Problems*, Vol. 25, March 2009, doi: 10.1088/0266-5611/25/3/03500.
9. C Lieberman, “Parameter and State Model Reduction for Bayesian Statistical Inverse Problems,” SM Thesis, MIT, February 2009.
10. C Lieberman, K Willcox, O Ghattas, “Parameter and state model reduction for large-scale statistical inverse problems,” *SIAM Journal on Scientific Computing*, Vol. 32, No. 5, pp. 2523–2542, August 2010.

11. Y Marzouk, D. Xiu, “A stochastic collocation approach to Bayesian inference in inverse problems,” *Communications in Computational Physics*, Vol. 6, pp. 826–847, 2009.
12. Y Marzouk, H Najm, “Dimensionality reduction and polynomial chaos acceleration of Bayesian inference in inverse problems,” *Journal of Computational Physics*, Vol. 228, pp. 1862–1902, 2009.
13. *Computational Methods for Large-Scale Inverse Problems and Quantification of Uncertainty*, L. Biegler, G. Biros, O. Ghattas, M. Heinkenschloss, D. Keyes, B. Mallick, Y. Marzouk, L. Tenorio, B. van Bloemen Waanders, K. Willcox (Eds.), Wiley Series in Computational Statistics, January 2011.
14. M. Frangos, Y. Marzouk, K. Willcox, B. van Bloemen Waanders, “Surrogate and reduced-order modeling: a comparison of approaches for large-scale statistical inverse problems,” in *Computational Methods for Large-Scale Inverse Problems and Quantification of Uncertainty*, Biegler et al. (Eds.), Wiley Series in Computational Statistics, January 2011.
15. H.P. Flath, L.C. Wilcox, V. Akcelik, J. Hill, B. van Bloemen Waanders, and O. Ghattas, Fast algorithms for Bayesian uncertainty quantification in large-scale linear inverse problems based on low-rank partial Hessian approximations, *SIAM Journal on Scientific Computing*, 33(1):407-432, 2011.
16. C. Lieberman, K. Fidkowski, K. Willcox, B. van Bloemen Waanders, “Hessian-based model reduction: Large-scale inversion and prediction,” *International Journal of Numerical Methods in Fluids* Vol. X, No. Y, pp. xx–xx, 2012.
17. T. Bui-Thanh, C. Burstedde, O. Ghattas, J. Martin, G. Stadler, and L.C. Wilcox, Extreme-scale UQ for Bayesian inverse problems governed by PDEs, *Proceedings of IEEE/ACM SC12*, 2012
18. C. Lieberman and K. Willcox, Goal-Oriented Inference: Approach, Linear Theory, and Application to Advection Diffusion. *SIAM Review*, 55-3, 493–519, 2013. Also *SIAM Journal on Scientific Computing*, Vol. 34, Np. 4, pp. 1880–1904, 2012.
19. T. Bui-Thanh, O. Ghattas, and D. Higdon, Adaptive Hessian-based non-stationary Gaussian process response surface method for probability density approximation with application to Bayesian solution of large-scale inverse problems, *SIAM Journal on Scientific Computing*, 34(6):A2837A2871, 2012.
20. Goal-oriented inference: Theoretical foundations and application to carbon capture and storage. C. Lieberman, Ph.D. Thesis, Aeronautics and Astronautics, Massachusetts Institute of Technology, June 2013.
21. H. Pearl Flath, Hessian-based response surface approximations for uncertainty quantification in large-scale statistical inverse problems, with applications to groundwater flow, Ph.D. Thesis, Computational Science, Engineering, and Mathematics, University of Texas at Austin, August 2013.

Talks

1. Y Marzouk, “Uncertainty and Bayesian inference in inverse problems,” ASC Verification & Uncertainty Quantification seminar series, Lawrence Livermore National Laboratory, Livermore, CA, September 2008.
2. O Ghattas, “Stochastic Newton MCMC for sampling expensive probability densities in high dimensions,” Center for Applied Scientific Computing Seminar, Lawrence Livermore National Laboratory, Livermore, CA, October 2008.
3. O Ghattas, “Bridging deterministic and stochastic approaches in the solution of large-scale PDE-based statistical inverse problems,” DOE Advanced Scientific Computing Advisory Committee, Gaithersburg, MD, October 2008.
4. K Willcox, “Uncertainty Quantification and Optimization of Complex Systems: The Challenge and Promise of Model Reduction,” Applied Mathematics Principal Investigators Meeting, Argonne National Laboratory, Argonne, IL, October 2008.
5. K Willcox, “Model Reduction for Design, Control and Probabilistic Analysis of Large-Scale Systems,” Norwegian University of Science and Technology, Trondheim, Norway, October 2008.
6. O Ghattas, “A stochastic Newton method for large-scale Bayesian inverse problems,” Oberwolfach Workshop on Numerical Techniques for Optimization Problems with PDE Constraints, Oberwolfach, Germany, January 2009.
7. O Ghattas, “Exploiting PDE Problem Structure in Large-Scale Statistical Inverse Problems,” New Zealand Institute for Mathematics and its Applications, Programme in Energy, Wind and Water: Algorithms for Simulation, Optimization and Control, Auckland, New Zealand, February, 2009.
8. C Lieberman, “Reduced-order modeling for statistical inverse problems in groundwater flows,” New Zealand Institute for Mathematics and its Applications, Programme in Energy, Wind and Water: Algorithms for Simulation, Optimization and Control, Auckland, New Zealand, February, 2009.
9. G Biros, “,” SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
10. C Dawson, “An Iterative Representer-Based Scheme for Data Inversion in Reservoir Modeling,” SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
11. P Flath, “Fast Algorithms for Uncertainty Estimation and Propagation in Large Scale Linear Dynamical Systems,” SIAM Conference on Computational Science and Engineering, Miami, FL, March 2009.
12. O Ghattas, “An introduction to PDE-based statistical inverse problems, Uncertainty Quantification Mini-tutorial,” SIAM Conference on Computational Science and Engineering, Miami, FL, March 2009.
13. O Ghattas, Computational Science and Engineering Forward Looking Panel, SIAM Conference on Computational Science and Engineering, Miami, FL, March 2009.

14. C Lieberman, "Model Reduction for Uncertainty Quantification in Large-scale Inverse Problems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
15. J Martin, "A Stochastic Newton Method for Bayesian Inverse Problems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
16. Y Marzouk, "Stochastic collocation and Galerkin methods for Bayesian inverse problems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
17. Y Marzouk, "Nonparametric Bayesian density estimation in hierarchical engineered systems," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
18. K Willcox, "Model Reduction for Uncertainty Quantification and Decision-Making Under Uncertainty," SIAM Conference on Computational Science and Engineering (invited minisymposium), Miami, FL, March 2009.
19. Y Marzouk, "Uncertainty Quantification and Statistical Inference in Computational Engineering," RWTH-Aachen, Institute for Advanced Study in Computational Engineering Science (AICES), Aachen, Germany, March 2009.
20. K Willcox, "Model Reduction for Uncertainty Quantification in Large-Scale Complex Systems," Seminar Series in Verification, UQ and Sensitivity Analysis, Lawrence Livermore National Laboratory, Livermore, CA, May 2009.
21. K Willcox, "Model Reduction for Uncertainty Quantification and Optimization of Large-Scale Systems," Plenary Talk, SIAM Conference on Applied Linear Algebra, Monterey Bay-Seaside, CA, October 2009.
22. K Willcox, "Model Reduction for Uncertainty Quantification and Optimization Under Uncertainty of Complex Systems," Workshop on Computing with Uncertainty, Institute for Mathematics and its Applications (IMA), Minneapolis, MN, October 2010.
23. K Willcox, "Model Reduction for Design, Optimization, Inverse Problems and Quantification of Uncertainty in Large-scale Systems," Singapore-Delft Water Alliance, Singapore, March 2011.
24. K Willcox, "Surrogate and Multifidelity Modeling for Optimization Under Uncertainty of Large-scale Complex Systems," Aachen Conference on Computational Engineering Science, Aachen, Germany, July 2011.
25. K Willcox, "Model Reduction for Large-Scale Systems: Efficient Approaches for Problems with High-Dimensional Parameter Spaces," Peaceman Lecture on Numerical Mathematics, Rice University, Houston, TX, September 2011.
26. K Willcox, "Model Reduction and Surrogate Modeling for Uncertainty Quantification," Statistical and Applied Mathematical Sciences Institute (SAMSI) 2011-12 Uncertainty Quantification Program Methodology Opening Workshop, Research Triangle Park, NC, September 2011.

27. K Willcox, "Model Reduction for Large-Scale Systems: Efficient Approaches for Problems with High-Dimensional Parameter Spaces," Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, October 2011.
28. K Willcox, "Model reduction for uncertainty quantification of large-scale systems," Plenary talk, SIAM Conference on Uncertainty Quantification, Raleigh, NC, April 2012.
29. K Willcox, "Multifidelity Modeling for Identification, Prediction and Optimization of Large-Scale Complex Systems," Plenary talk, SIAM Annual Meeting, Minneapolis, MN, July 2012.
30. K Willcox, "Model reduction for uncertainty quantification of large-scale systems," Special AIAA-SIAM Session on Uncertainty Quantification and Management for Complex Systems, AIAA Multidisciplinary Analysis and Optimization Conference, Indianapolis, IN, September 2012.
31. K Willcox, "Model reduction for systems with high-dimensional parameter spaces," Seminar for Applied Mathematics, ETH Zurich, Switzerland, October 2012.
32. K Willcox, "Model Reduction: Exploiting Structure in Large-Scale Complex Systems," Plenary Talk, MathBio4: Scale Symposium, Madison, WI, October 2012.
33. K Willcox, "Model reduction for systems with high-dimensional parameter spaces," Applied and Computational Math Seminar, George Mason University. Also Numerical Analysis Seminar, University of Maryland, November 2012.
34. O. Ghattas, Uncertainty quantification for large scale inverse problems, with applications to seismic inverse problems, Uncertainty in Computer Models 2012, Sheffield, UK, July 24, 2012.
35. O. Ghattas, Toward uncertainty quantification in large-scale Bayesian inverse problems, with geophysical applications, 8th Erlangen International High-End-Computing Symposium, Erlangen, Germany, June 22, 2012.
36. O. Ghattas, Uncertainty quantification in geophysical inverse problems: Opportunities and challenges, Winter Enrichment Program, KAUST, January 14, 2012.
37. O. Ghattas, Grand challenges in computational inverse problems, with illustrations from geophysics, Challenges in Computing, Oslo, December 1415, 2011.
38. O. Ghattas, A stochastic Newton method for large-scale seismic wave propagation inverse problems, 10th International Conference on Mathematical and Numerical Aspects of Waves Propagation (WAVES 2011), Vancouver, Canada, July 2529, 2011.
39. O. Ghattas, Extreme-scale UQ for inverse problems, TACC Booth, SC12, Salt Lake City, UT, November 14, 2012.
40. O. Ghattas, Large scale Bayesian solution of seismic inverse problems, Oberwolfach meeting on computational inverse problems, Oberwolfach Institute, Germany, October 2226, 2012
41. O. Ghattas, Extreme-scale UQ for inverse problems, with applications to global seismic inversion, Uncertainty Quantification for High-Performance Computing, Oak Ridge National Laboratory, Oak Ridge, TN, May 24, 2012.
42. O. Ghattas, Toward extreme scale stochastic inversion, SIAM Conference on Uncertainty Quantification, Raleigh, NC, April 14, 2012.

43. O. Ghattas, Research directions in verification, validation, & uncertainty Quantification, National Academies Symposium on Verification, Validation, and Uncertainty Quantification, National Research Council, Washington, DC, March 28, 2012.
44. O. Ghattas, Uncertainty quantification in full waveform seismic inversion, Texas Consortium for Computational Seismology 2012 Spring Research Meeting, Houston, TX, March 23, 2012.
45. O. Ghattas, Large-scale parallel Hessian-based methods for uncertainty quantification in inverse problems, SIAM Conference on Parallel Processing for Science and Engineering, Savannah, GA, February 15-17, 2012.
46. O. Ghattas, Uncertainty quantification for large-scale inverse problems: Challenges and opportunities, First Annual CESM Uncertainty Quantification and Analysis Interest Group Meeting, NCAR, Boulder, CO, January 30, 2012.
47. O. Ghattas, Large Scale Uncertainty Quantification for Stochastic Inverse Problems with Applications to Seismic Inversion, Colloquium on Advances in Computational Science, Engineering and Mathematics, Austin, Texas, January 19-21, 2012.
48. O. Ghattas, Hessian-based reduction for large-scale statistical inverse wave propagation, Workshop on Fast Solvers for Simulation, Inversion, and Control of Wave Propagation Problems, Wurzburg, Germany, September 26-28, 2011.
49. O. Ghattas, A stochastic Newton method for large-scale statistical inverse problems with application to geophysical inverse problems, SAMSI Program on Uncertainty Quantification: Geosciences, Research Triangle Park, NC, September 21-23, 2011.
50. O. Ghattas, Large-scale seismic inversion: elastic-acoustic coupling, DG discretization, gradient consistency, adaptivity, uncertainty quantification, and parallel algorithms, ICIAM 2011, Vancouver, Canada, July 18-22, 2011.
51. O. Ghattas, Uncertainty quantification for large-scale full-Stokes ice sheet modeling and simulation, ICIAM 2011, Vancouver, Canada, July 18-22, 2011.
52. O. Ghattas, Scalable algorithms for large-scale statistical inverse problems, with application to global seismic inversion, Aachen Conference on Computational Engineering Science, Aachen, Germany, July 13-15, 2011.
53. O. Ghattas, Top Five Grand Challenges in Computational Science, TACC 10th Anniversary Celebration, Austin, TX, June 24, 2011.
54. O. Ghattas, The role of TACC in enabling research on multiscale geophysical problems, TACC 10th Anniversary Celebration, Austin, TX, June 24, 2011.
55. O. Ghattas, A stochastic Newton method for large-scale statistical inverse problems, with application to seismic inversion, Inverse Problems and Optimal Control for PDEs, Warwick, UK, May 23-27, 2011.
56. O. Ghattas, Large-scale seismic inversion: elastic-acoustic coupling, DG discretization, gradient consistency, adaptivity, uncertainty quantification, and parallel algorithms, Workshop on Multiscale Modeling, Advanced Discretization Techniques, and Simulation of Wave Propagation, KAUST, Saudi Arabia, May 7-8, 2011.

57. O. Ghattas, DG-based, UQ-equipped, parallel, adaptive, scalable elastic-acoustic seismic inversion, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Long Beach, CA, March 21-24, 2011.
58. O. Ghattas, O. Ghattas, Grand Challenges for Next Generation End-to-End Earthquake Simulations: Uncertainty Quantification and Exascale Computing, National Research Council Workshop on Grand Challenges in Earthquake Engineering Research, The Beckman Center of the National Academies, March 14-15, 2011.
59. O. Ghattas, A Stochastic Newton Method for Large-scale Statistical Inverse Problems with Application to Geophysical Inverse Problems, SIAM Conference on Computational Science and Engineering, Reno, NV, February 28-March 4, 2011.
60. O. Ghattas, Acceleration of MCMC for high dimensional statistical inverse problems via reduction of parameter-to-observable maps, Reduction Strategies for the Simulation of Complex Problems, Milan, Italy, January 19-21, 2011.
61. O. Ghattas, Uncertainty quantification with advanced ice sheet models, Land Ice Working Group meeting, National Center for Atmospheric Research, Boulder, CO, January 12-13, 2011.
62. O. Ghattas, A stochastic Newton method for statistical inverse problems governed by PDEs, Joint IMS-ISBA Meeting (MCMSki3), Park City, Utah, January 5-7, 2011.
63. O. Ghattas, A stochastic Newton method for large-scale statistical inverse problems, 1st Joint North American Meeting on Industrial and Applied Mathematics, Huatulco, Mexico, December 7-10, 2010.
64. O. Ghattas, Uncertainty quantification and dynamic data-driven application systems, Panel on Infosymbiotic Systems, SC10, New Orleans, November 16, 2010.
65. O. Ghattas, Extreme scale AMR, TACC Booth, SC10, New Orleans, November 16, 2010.
66. O. Ghattas, A stochastic Newton method for large-scale statistical inverse problems, INFORMS Annual Meeting, Austin, Texas, November 7-10, 2010.
67. O. Ghattas, Towards exascale computing for uncertainty quantification in geophysical inverse problems, NSF Workshop on Application Drivers for Exascale Computing and Data Cyberinfrastructure, Arlington, Virginia, July 29, 2010.
68. O. Ghattas, Uncertainty Quantification for Large-Scale Inverse Scattering, AFOSR Computational Mathematics Program Review, Arlington, VA, July 28, 2010.
69. O. Ghattas, Opportunities and challenges for uncertainty quantification in large-scale models, NSF Workshop on Land-Ice Contributions to Sea Level, Sterling, VA, July 11, 2010.
70. O. Ghattas, Large-Scale Optimization for Bayesian Inference in Complex Systems, DOE Applied Mathematics Program Meeting, Berkeley, CA, May 4, 2010.
71. O. Ghattas, A stochastic Newton method for statistical inverse problems, with application to inverse scattering, KAUST Source Inversion Workshop, KAUST, Thuwal, Saudi Arabia, March 22-24, 2010.

72. O. Ghattas, Advanced computational methods for large-scale forward and inverse ice sheet dynamics, Community Climate System Model Land Ice Working Group Winter Meeting, Boulder, CO, February 17, 2010.
74. O. Ghattas, Implications for HPC from the perspective of PDE-based modeling in the evolution from simulation to simulation-based inference, prediction, and decision-making, NSF Workshop on Community Input on the Future of High-Performance Computing, Arlington, Virginia, December 4, 2010.
75. O. Ghattas, A stochastic Newton method for statistical inverse problems governed by PDEs, SIAM Annual Meeting, Denver, CO, July 610, 2009.
76. O. Ghattas, An introduction to PDE-based statistical inverse problems, Uncertainty Quantification Minitutorial, SIAM Conference on Computational Science and Engineering, Miami, FL, March 26, 2009.
77. O. Ghattas, Scalable adaptive mantle convection simulation on petascale supercomputers, SIAM Conference on Computational Science and Engineering, Miami, FL, March 26, 2009.
78. O. Ghattas, Computational Science and Engineering Forward Looking Panel, SIAM Conference on Computational Science and Engineering, Miami, FL, March 26, 2009.
79. O. Ghattas, A stochastic Newton method for large-scale Bayesian inverse problems, with application to geophysical inverse problems, Workshop on Energy, Wind and Water: Algorithms for Simulation, Optimization and Control, The New Zealand Institute of Mathematics and its Applications, Auckland, New Zealand, February 912, 2009.
80. O. Ghattas, A stochastic Newton method for large-scale Bayesian inverse problems, Oberwolfach Workshop on Numerical Techniques for Optimization Problems with PDE Constraints, Oberwolfach, Germany, January 2531, 2009.
81. O. Ghattas, Large Scale Bayesian Inverse Problems, with Applications to Seismic Inversion, Department of Applied Mathematics & Statistics Colloquia, Colorado School of Mines, Golden, CO, September 21, 2012.
82. O. Ghattas, Uncertainty Quantification in Large Scale Seismic Inverse Problems, CSRI Seminar, Sandia National Laboratories, Albuquerque, NM, June 4, 2012.
83. O. Ghattas, Uncertainty Quantification in Geophysical Inverse Problems: Opportunities and Challenges, Departamento de Matematica, Escuela Politecnica Nacional, Quito, Ecuador, March 16, 2012.
84. O. Ghattas, Large-scale stochastic inversion, with application to global seismic inversion, Sandia National Laboratories, Livermore, CA, December 2, 2011.
85. O. Ghattas, A Stochastic Newton Method For Large-Scale Statistical Inverse Problems, MIT Computational Engineering Seminar Series, Massachusetts Institute of Technology, Cambridge, MA, May 12, 2010.
86. O. Ghattas, Towards Uncertainty Quantification for Large-scale Inverse Problems, Robert J. Melosh Medal Competition for Best Student Paper in Finite Elements, Duke University, Durham, NC, April 30, 2010.

87. O. Ghattas, Stochastic Newton Method for Statistical Inverse Problems Governed by PDEs, National Center for Atmospheric Research, Boulder, CO, May 19, 2009.
88. O. Ghattas, Bridging deterministic and stochastic approaches in the solution of large-scale PDE-based statistical inverse problems, DOE Advanced Scientific Computing Advisory Committee, Gaithersburg, MD, October 28, 2008.
89. O. Ghattas, Stochastic Newton MCMC for sampling expensive probability densities in high dimensions, Center for Applied Scientific Computing Seminar, Lawrence Livermore National Laboratory, Livermore, CA, October 10, 2008.

Awards

1. Finalist, *2008 ACM/IEEE Gordon Bell Prize* for the paper “Scalable parallel mantle convection simulation on petascale computers,” C. Burstedde, O. Ghattas, M. Gurnis, G. Stadler, E. Tan, T. Tu, L. Wilcox, S. Zhong, SC2008, Austin, TX, Nov. 2008
2. C. Lieberman (graduate student, MIT) received second place in the Bavarian Graduate School of Computational Engineering (BGCE) Student Paper Prize for outstanding student work in the field of Computational Science and Engineering, for his paper and presentation titled “Parameter and state model reduction for uncertainty quantification in large-scale statistical inverse problems.” Awarded March 2009 at the SIAM Conference on Computational Science and Engineering, Miami, FL.
3. C. Lieberman and K. Willcox received a SIGEST Award from SIAM for their paper “Goal-Oriented Inference: Approach, Linear Theory, and Application to Advection Diffusion.”
4. Selection of the paper T. Bui-Thanh and O. Ghattas, “Analysis of the Hessian for inverse scattering problems: I. Inverse shape scattering of acoustic waves” for the 2012 Highlights of the journal *Inverse Problems*.
5. O. Ghattas, 2012 Joseph C. Walter Excellence Award, Jackson School of Geosciences.
6. Finalist, 2012 Gordon Bell Prize, for the paper T. Bui-Thanh, C. Burstedde, O. Ghattas, J. Martin, G. Stadler, and L.C. Wilcox, “Extreme-scale UQ for Bayesian inverse problems governed by PDEs,” *Proceedings of ACM/IEEE SC12*, November 2012.
7. Finalist, 2010 Gordon Bell Prize, for the paper C. Burstedde, O. Ghattas, M. Gurnis, T. Isaac, G. Stadler, T. Warburton, L.C. Wilcox, “Extreme-Scale AMR,” *Proceedings of ACM/IEEE SC10*, November 2010.
8. Selection of the paper O. Ghattas et al., “A Newton-CG method for large-scale three-dimensional elastic full-waveform seismic inversion” in the 2008 Highlights of the journal *Inverse Problems*.