Final Report: DOE-USC-6833-1

DOE Award Number: DE-SC0006833

Recipient: University of Southern California

Project Title: Quantification of Uncertainty in Extreme Scale Computations (QUEST)

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Date: April 7 2017

Period Covered: 1 September 2012 – 31 December 2016

Broad Objectives

QUEST was a SciDAC Institute comprising Sandia National Laboratories, Los Alamos National Laboratory, the University of Southern California, the Massachusetts Institute of Technology, the University of Texas at Austin, and Duke University. The mission of QUEST is to: (1) develop a broad class of uncertainty quantification (UQ) methods/tools, and (2) provide UQ expertise and software to other SciDAC projects, thereby enabling/guiding their UQ activities.

The USC effort centered on the development of reduced models and efficient algorithms for implementing various components of the UQ pipeline. USC personnel were responsible for the development of adaptive bases, adaptive quadrature, and reduced models to be used in estimation and inference.

Summary of Work and Accomplishments

Development and implementation were made along three fronts, namely algorithmic, modeling, and mathematical. On the algorithmic side, we developed basis adaptation algorithms to tackle the curse of dimensionality in very large scale systems. We also developed convergence acceleration methods based on sequence transformations. On the modeling side, we devleoped the conceptual and mathematical ingredients for tackling variational inequality problems, crucial for the proper analysis of many problems of interest to DOE. On the mathematical side, we developed stochastic differential equation whose invariant solutions are concentrated on diffusion manifolds. Several of these developments are described below.

- **Basis Adaptation:** Much of the complexity in stochastic analysis which is typically attributed to the curse of dimensionality stems from the effort to characterize outputs from computational models as stochastic processes. This is a characterization in infinite dimensional space, and any L_2 characterization is bound, as such, to skirt with the curse of dimensionality. Recognizing that in many instances QoIs are lower dimensional objects, such as random variables, we have developed a procedure for basis discovery and adaptation that permits very efficient and accurate approximation within a subspace in which the QoI is concentrated. To achieve that, we rely on the mathematical structure of Gaussian Hilbert spaces and the associated Homogeneous Chaos space obtained from them through a tensor product construction, to obtain a reduced model that, while capturing the probabilistic content of the QoI, characterizes its functional dependence on the original parameterization. We have demonstrated the methodology on steady state problems, and are currently in the process of extending it as a general purpose approach for parameterized stochastic upscaling.

This can be important for carrying out deterministic and stochastic sensitivity analyses and worth of information studies. The approach hinges on Gaussian parameterization of the problem. This does not signify that the parameters in the problem are assumed to be Gaussian, but rather that they are functions of some underlying Gaussian variables or processes. In a first step, an isometry is applied to an underlying Gaussian variables to induce a particular desired structure in the representation of the solution. In a second step, a reduction through projection of the resulting representation is carried out that has a probabilistic interpretation, thus providing further justification for the algebraic manipulations. We have demonstrated the methodology on steady state problems, and are currently in the process of extending it as a general purpose approach for parameterized stochastic upscaling.

- **Conditional Polynomial Representations**

  we continue work on conditional polynomial representations as a means for implementing conditioning for problems whose solution has already been computed via polynomial chaos representations. Within the context of probability theory, standard updating is carried out using Bayes rule, which is a relationship between probability density functions. The likelihood, which is the part of Bayes rule that expresses the dependence of two random variables on each other, only expresses the probability of one random variable given the other. The likelihood is agnostic to the functional dependence between the two random variables. In many instances in computational science, we do in fact have a deterministic structure to the map from one random variable onto another. This is the case for instance where the map is a deterministic operator with random coefficients. In these cases, it would appear that Bayes theorem is not capitalizing on all the information used to construct our problem. We have developed an updating procedure that works directly in L_2 space. Thus, given that an L_2 characterization has been achieved, in the form of a polynomial chaos representation, we update it without having to pass through probability densities. The updating is construed as stabilization or equivalently as projection onto a suitable set. We are currently exploring the mathematical properties of these projections and the characters of the projection sets for which mathematical statements can be made. One paper detailing this effort is in the final stages of preparation. As a by-product of this project, in light of using data provided by PNNL, we developed algorithms for applications in smart grid management, published in the paper by Bassamzadeh et.al (2015).

- **Stochastic Variational Inequalities (SVI**

  An important challenge in the computational analysis of many physical processes pertains to inequality constraints. These are encountered in the modeling of material undergoing phase transformations, in the interaction of components undergoing contact, as well as in the characterization of processes on networks and graphs. Describing these constraints in the form of variational inequalities puts them in a mathematical form that is readily amenable to stochastic analysis via stochastic projection formalisms and polynomial chaos machinery. We are pursuing two approaches to the SVI problem. In a first approach, we are discretizing the variational form using sparse quadrature. This extends previous work by Ghanem and Arnst on this problem. In a second approach, we developed methods from semi-infinite programming that are very-well suited to this class of problems.

- **Stochastic Processes on Manifolds**

  Characterizing the probabilistic content of stochastic processes is accentuated when they are defined on arbitrary manifolds, instead of throughout a vector space. An important case that was addressed in a recent paper (Soize and Ghanem, 2015) considers the case when this manifold is the manifestation of a manufacturing process that induces a variety of changes to the physical object underlying the observed uncertainty. The changes are described as nonlinear mappings and we investigate the relationship between the properties of these mappings and the statistical properties of the transformed physical device. We thus consider mappings that, while modifying the geometry of the object, leaves its microstructure intact. We note that even in this case, the second order statistical properties of the deformed material can be quite distinct of the original properties, depending on the magnitude of the geometric deformation. We then consider the impact of nonlinear mappings that induce a random transformation in the microstructure of the material, which is very typical of most manufacturing processes. In this case, no matter how simplistic the manufacturing process is, the effect on the statistics of the transformed material is very significant, requiring consideration of the mechanics of the manufacturing process and the introduction of a corresponding mathematical model.

  Another important case where stochastic processes on manifolds are manifest is in situations where these manifolds are detected, through various dimension reduction and embedding techniques. In these cases, a rigorous restriction, to the manifold, of the original stochastic process, described in the whole space, is required. Stochastic evolutions and polynomial chaos expansions on these manifolds must also be enabled. A challenge in these cases is that the number of samples on the manifold may be too small to carry out estimation in the whole space. Our interest in this problem had its genesis in an application of nested polynomial chaos expansions to a NETL funded project on "Confident Predictions of Reservoir and Well Bore Flow using Reduced Models and Data," partial results from which are published in Charan et.al (2015). In that work, a polynomial chaos representation, followed by a high-dimensional (36-dimensions) Gaussian process interpolation of the polynomial chaos coefficients permitted a credible assessment of gas production at new sites in the Gulf of Mexico. The results were further refined when the Gaussian process interpolation was described in terms of a diffusion metric associated with a low-dimensional manifold embedded in the 36-dimensional space. That work is currently being expanded, under QUEST, to permit the construction of probability measures with support restricted to the low dimensional manifold. This restriction (which is really a form of extrinsic knowledge) permits us to augment any database with statistically consistent realizations. The structure of the manifold is learned by considering as building blocks for the statistical analysis, not each single observation, but rather a number of observations scattered along the manifold. The probabilistic construction then aims at developing a probability measure for the random matrix thus synthesized, its rows indexing the dimensions, and its columns indexing the observations. This work is a collaboration with Professor C. Soize and two papers detailing the theory and application have already appeared in JCP.

Impact on other DOE-funded work

- USC and QUEST-developed algorithms have been used in a NETL-funded contract entitled "Confident Predictions of Reservoir and Well Bore Flow using Reduced Models and Data." This project develops reduced order models for deep sea reservoirs and deep sea wellbores. It also integrates these two reduced models with an eye towards assessing the risks associated with future deep sea drilling operations as well as quantifying the fluxes at the seafloor following an accident.
- USC and QUEST-developed algorithms are also making significant impact on a recent collaboration with General Motors aimed at developing lightweight vehicles. That effort is funded by DOE under DE-FOA-0000991 (ICME Development of Carbon Fiber Composites for Lightweight Vehicles) and is entitled "Development and Integration of Predictive Models for Manufacturing and Structural Performance of Carbon Fiber Composites in Automotive Applications." USC's role in that effort is the development of stochastic models and of algorithms for the integration and coupling of predictive tools for material processing and manufacturing and for assembly and production.

Publications/Presentations

Journal Publications:

1. Ghanem, R., Soize, C., and Thimmisetty, C., "Efficient probabilistic optimization for well placement in heterogeneous random subsurface," submitted, *SPE Journal*, 2017.
2. Soize, C. and Ghanem, R. "Data-driven probability concentration and sampling on manifold," *Journal of Computational Physics,* Vol. 321, pp. 242-258, 2016.
3. Ghanem, R. and Soize, C., "Remarks on stochastic properties of materials through finite deformations", *Journal of Multiscale Computational Engineering,* Vol. 13, No. 4, pp. 367-374, 2015.
4. Thimmisety, C., Ghanem, R., Khodabakhsh, A., Jabbari, N., Aminzaddeh, F., Rose, K., DIenhof, C., and Bauer, J., "Multiscale Stochastic Representation in High-Dimensional Data using Gaussian Processes with Implicit Diffusion Metrics," *Lecture Notes in Computer Science, LNCS 8964*, 2015.
5. Ghanem, R., Yadegaran, I., Thimmisetty, C., Keshavarzzadeh, V., Masri, S., Red-Horse, J., Moser, R., Oliver, T., Spanos, P., and Aldraihem, O., "A Probabilistic Approach to the NASA Langley Multidisciplinary Uncertainty Quantification Challenge Problem," *AIAA Journal of Aerospace Information Systems,* Vol. 12, pp. 170-188, 2015 (doi: 10.2514/1.I010271 .)
6. Bassamzadeh, N., Ghanem, R., Lu, S. and Kazemitabar, J., "Robust scheduling of smart appliances with uncertain electricity prices in a heterogeneous population," *Energy and Buildings,* Vol. 84, pp. 537-547, 2014.
7. Mehrez, L., Darabi, M., Ghanem, R., Masad, E., and Little, D., "Modeling and Propagation of Stochastic Linear Viscoelastic Material Properties of Asphalt Mixtures in Pavement Structures," *EURODYN 2014, The Ninth International Conference on Structural Dynamics,* Porto, Portugal, June 30 - July 2 2014.

8. Mehrez, L., Ghanem, R., and Masad, E., "A spectral stochastic framework for the uncertainty quantification of asphalt mixture behavior," *EMI2014: Engineering Mechanics Institute Conference,* McMaster University, Hamilton, ON, August 5-8, 2014.

9. Comboul, M. and Ghanem, R., "Multiscale Modeling for Stochastic Forest Dynamics," in press, *International Journal for Multiscale Computational Engineering,* 2014.

10. Meidani, H. and Ghanem, R., "Spectral power iterations for the random eigenvalue problem," *AIAA Journal,* Vol. 52, o. 5, pp. 912-925, 2014.

11. Sousedik, B. and Ghanem, R., "Truncated hierarchical preconditioning for the stochastic Galerkin FEM," in press, *International Journal on Uncertainty Quantification,* 2014.

12. Tipireddy, R. and Ghanem, R. "Adaptation in homogeneous chaos spaces," *Journal of Computational Physics,* Vol. 259, pp. 304-317, 2014.

13. V. Keshavarzzadeh, R. Ghanem , S. Masri and O. Aldraihem, "Convergence acceleration of polynomial chaos solutions via sequence transformation," *Computer Methods in Applied Mechanics and Engineering,* Vol. 271, No. 1, pp. 167-184, 2014.

14. Sousedik, B., Ghanem, R., and Phipps, E., "Hierarchical Schur complement preconditioner for the stochastic Galerkin finite element methods," *Numerical Linear Algebra with Applications,* Vol. 21, No. 1, pp. 136-151, 2014.

15. Arnst, M., Ghanem, R., Phipps, E., and Red-Horse, J., "Reduced chaos expansions with random coefficients in reduced-dimensional stochastic modeling of coupled problems," *International Journal for Numerical Methods in Engineering,* Vol. 97, No.5., pp. 352-376, 2014.

16. Arnst, M., Soize, C., and Ghanem, R., "Hybrid sampling/spectral method for solving stochastic coupled problems," *SIAM/ASA Journal on Uncertainty Quantification,* Vol. 1, No. 1, pp. 218-243, 2013.

17. Ghanem, R., Thimmisetty, C., Yadegaran, I., Keshavarzzadeh, V., Masri, S., Red-Horse, J., Moser, R., Oliver, T., Spanos, P., and Aldreiham, O., "A Probabilistic Approach to the NASA Langley Multidisciplinary Uncertainty Quantification Challenge Problem," *16th AIAA Non-Deterministic Approaches Conference,* National Harbor, MD January 14-17, 2014.

Keynote Lectures:

18. "Uncertainty Quantification for Complex Interacting Systems," *6^{th} Asian Pacific Symposium on Structural Reliability and its Applications,* Shanghai, China, May 28-30 2016.

19. "Uncertainty Modeling and Quantification for Complex Decisions," (keynote) *First International Conference on the Quantification of Uncertainty in Engineering, Science and Technology (QUEST)*, Beihang University, Beijing, China, October 19-23, 2015.

20. "Risk Assessment for Complex Systems," (keynote) ASCE Engineering Mechanics Institute Inaugural International Conference, Hong-Kong Polytechnic University, January 7-9 2015.

21. R. Ghanem (Keynote lecture) "Stochastic Model Reduction with Basis and Measure Adaptation," *Aachen Conference on Computational Engineering Science,* Aachen, Germany, September 9 2013.

22. R. Ghanem (Keynote lecture) "Stochastic Reduced Models," *EURODYN 2014, The Ninth International Conference on Structural Dynamics,* Porto, Portugal, June 30 - July 2 2014.

23. R. Ghanem (Keynote lecture) "Stochastic Model Reduction with Basis and Measure Adaptation," *Aachen Conference on Computational Engineering Science,* Aachen, Germany, September 9 2013.

Conferences:

24. Ghanem, R., Mehrez, L., Thimmisetty, C., Aitharaju, V., Rodgers, W., Fish, J." "Stochastic methods for upscaling material properties and behavior with application to composites," *Society of Engineering Science (SES) Conference,* College Park, MD October 5, 2016.

25. Jianyu, L. and Ghanem, R., "Numerical solution method for stochastic variational inequalities with polynomial chaos decompositions," *19th European Conference on Mathematics for Industry,* June 16, 2016, Santiago de Compostela, Spain.

26. Li, J. and Ghanem, R., "Stochastic variational inequalities with polynomial chaos," *The 8th International Congress on Industrial and Applied Mathematics,* Beijing, China, August 10-14 2015.

27. Li, J. and Ghanem, R.. "Two Approaches for Solving Stochastic Variational Inequality Problems in the Framework of Polynomial Chaos Expansions," *13th US National Congress on Computational Mechanics,* LaJolla, CA, July 26-30 2015.

28. Ghanem, R., Tipireddy, R., Chowdhary, K., and Najm, H., "QoI basis adaptation," *SIAM Conference on Computational Science and Engineering,* Salt Lake City, March 17 2015.

29. Ghanem, R. and Tipireddy, R. "Stochastic model reduction and multiscale modeling with uncertainty," *WCCM XI: World Congress on Computational Mechanics, Barcelona, Spain, July 23 2014.*

30. Haddad-Zadegan, H., Ghanem, R., and Hajali, P., "Data worth analysis in spatial prediction and soil remediation," *ICOSSAR'13: International Conference on Structural Safety and Reliability,* New York City, NY, June 16-20, 2013.

31. Meidani, H. and Ghanem, R., "Uncertainty quantification of diffusion maps," *ICOSSAR'13: International Conference on Structural Safety and Reliability,* New York City, NY, June 16-20, 2013.

32. Ghanem, R. and Meidani, H., "Uncertainty Quantification and Decisions for Markovian Dynamics," *SIAM Conference on Applications of Dynamical Systems,* Snowbird, UT, March 21 2013.

33. Kalligiannaki, E. and Ghanem, R., "Projections on positive random variables in finite Wiener chaos spaces," *SIAM CS&E Conference,*, Boston, MA, February 25-March 1, 2013.

34. Tipireddy, R. and Ghanem, R., "Stochastic reduced models," *SIAM CS&E Conference,*, Boston, MA, February 25-March 1, 2013.

35. Ghanem, R. and Tipireddy, R., “Dimension reduction for the random eigenvalue problem,” *Advances in Computational Mechanics (ACM 2013),* San Diego, CA, February 24-27 2013.

36. Ghanem, R., “Model reduction in uncertainty quantification: An interplay between basis and measure adaptation,” (invited semi-plenary talk) *12th World Congress on Computational Mechanics,* Sao-Paolo, Brazil, July 8-13, 2012.

37. Ghanem, R., “UQ in Computational Science and Engineering,” (invited plenary talk) *Fourth International Conference on Scientific Computing and Partial Differential Equations (SCPDE11),* Hong Kong, China, December 5-9, 2011.

38. Meidani, H., and Ghanem, R., “Diffusion on Random Manifolds,” *2012 SIAM International Conference on Data Mining,* Anaheim, CA, April 26-28.

39. Das,S., Spall, J. and Ghanem, R. “Efficient Monte Carlo computation of Fisher information matrix using prior information,” *2012 SIAM International Conference on Data Mining,* Anaheim, CA, April 26-28.

40. Meidani, H. and Ghanem, R., “Maximum entropy construction for data-driven analysis of diffusion on random manifolds,” *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.

41. Arnst, M., Ghanem, R., Phipps, M., and Red-Horse, J., “Dimension reduction and measure transformation in stochastic multiphysics modeling,” *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.

42. Noshadravan, A., Ghanem, R., Guilleminot, J., Atodaria, I., and Peralta, P., “Validation of a random matrix model for mesoscale elastic description of materials with microstructures,” *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.

43. Sousedik, B., Ghanem, R., and Phipps, E., “Hierarchical Schur complement preconditioner for the stochastic Galerkin finite element methods,” *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.

44. Phipps, E., Arnst, M., Constantine, P., Ghanem, R., Red-Horse, J., and Wildey, T., “Stochastic Dimension Reduction Techniques for Uncertainty Quantification of Multiphysics Systems,” *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.

45. Ghanem, R. and Tipireddy, R., “Stochastic basis reduction via QoI adaptation,” *SIAM First Conference on Uncertainty Quantification,* Raleigh, NC, April 2-5, 2012.

46. Ghanem, R., “V&V or the Schizophrenia of Prediction Science: from Diagnosis to Therapy,” *MIT Distinguished Speaker Series in Computational Science and Engineering,* Cambridge, March 7 2012.

47. Ghanem, R., “A Perspective on Uncertainty Quantification and Model Validation,” Princeton University, April 9 2012.

48. R. Ghanem, (6-hour short course) “Stochastic Computational Science,” *SIAM Conference on Uncertainty Quantification,* Rayleigh, NC, April 1 2012.

49. R. Ghanem, (6-hour short course) "Stochastic Representations of Model-Based Predictions and Associated Data Assimilation," *CIMPA UNESCO School in Applied Mathematics,* KAUST, Saudi Arabia, Spring 2012.

50. R. Ghanem, "Model reduction in Stochastic PDEs," (invited talk) *NASPDE12 (Numerical Solution of Stochastic PDEs)*, Warwick, UK, June 11-12, 2012.

51. R. Ghanem, "Uncertainty in Reduced Order Models: A blessing or a curse ?" (invited talk) *Workshop on Reduced Basis, POD and PGD Model Reduction Techniques: a Breakthrough in Computational Engineering ?* Cachan, France, November 16-17-18, 2011.

52. "Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification," *NRC Committee on Mathematical Foundations of Verification, Validation, and Uncertainty Quantification*, 2012.

Workshops:

53. "Stochastic Modeling for Performance and Design Across Scales," *IUTAM Symposium on Materials under Extremes* June 20-22, 2016.

54. "Reliability in the Age of High Fidelity Sensors, Multiscale Models, and High-Performance Computing," *International Workshop on Engineering Reliability and Stochastic Mechanics (IWERSM 2016)*, Tongji University, Shanghai, June 1st 2016.

55. "Multiscale modeling in support of product design," *IMA Special Workshop on Optimization and Uncertainty Quantification in Energy and Industrial Applications,* Institute of Mathematics and Its Applications, February 22-24, 2016, University of Minnesota, Minneapolis, MN.

56. "Probabilistic Treatment of Multiscale Problems," *Workshop on Uncertainty Quantification in Multiscale Problems,* IPAM, UCLA, Los Angeles, January 19-22, 2016.

57. "Building Stochastic Models, One Constraint at a Time," *AFOSR/DARPA/NCI Strategic Workshop: Convergence of Physical Sciences for Biomedical Applications: Phase Transition and Network Dynamics in Living and Non-Living Systems*, Arlington, VA, August 28 2014.

58. Tipireddy, R. and Ghanem, R., "Basis Adaptation in UQ," *SIAM UQ Conference*, Savannah, GA, April, 2014.

59. R. Ghanem, "Stochastic Dimension Reductions and Cross-scale Representations," *2014 Albany User Group Meeting,* CSRI, Sandia National Laboratories, January 14-16 2014.

60. R. Ghanem, "Model Reduction and Synthesis for UQ," *Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2014)* , KAUST, January 6-10 2014.

61. R. Ghanem, "Uncertainty Quantification for Predictive Modeling of Materials," *ARO Workshop on Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials,* Johns Hopkins University, Baltimore, MD September, 5-6 2013.

62. R. Ghanem, "Stochastic Models for Coupled Physics,", *3^{rd} International Workshop on Moisture-Induced Damage in Asphalt Mixtures,* Doha, Qatar, April 16-19 2013.

63. R. Ghanem, "New directions in stochastic multiscale modeling," *Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization,* Mathematisches Forschungsinstitut Oberwolfach, Germany, March 1-23, 2013.

64. R. Ghanem, "Uncertainty Quantification," *Scientific Workflows for Scattering Science,* Caltech, Pasadena, CA January 31-February 2, 2013.

65. R. Ghanem, "Stochastic modeling and prediction for the design and management of interacting complex systems," *NSF Workshop on Building Engineering Complex Systems,* Arlington, VA, January 24-25, 2013.

66. R. Ghanem, "Linear solvers for tensorized spaces," *IMA Annual Program Year Workshop on Theory and Applications of Stochastic PDEs*, the Institute for Mathematics and Its Applications (IMA), University of Minnesota, January 14-18, 2013.

67. "Random field representations and approximations for fixed point iterations," *Computational and Theoretical Challenges in Interdisciplinary Predictive Modeling Over Random Fields,* Texas Tech University, Lubbock, TX, October 26, 2012.

Noteworthy Awards

- First prizes for students Hadi Meidani (2013) and Charan Thimmisetty (2014) in the Probabilistic Methods Committee student competitions, held during the Engineering Mechanics Annual meetings (New York City, and Hamilton, Canada, respectively).

- Ghanem is elected as AAAS fellow (2017).

- Ghanem is elected to executive council of the USACM, 2014-present.

- Ghanem served as president of Engineering Mechanics Institute of ASCE, 2011-2013.

- Ghanem elected Member *U.S. National Committee for Theoretical and Applied Mechanics,* 2014-present.

- Ghanem elected Chair of the *SIAM Activity Group (SIAG) on Uncertainty Quantification,* January 2017-present.

- Ghanem serves as member of the NRC Review Panel on Ballistics Science and Engineering at the Army Research Laboratory, 2015-present.

- Ghanem serves as member of the NRC Review Panel on Assessment and Analysis at the Army Research Laboratory, 2016.