# Final Technical Report

**DOE Award Number:** DE-SC0008789

**Recipient:** Duke University

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

**Principal Investigator:** Omar M. Knio
Department of Mechanical Engineering and Materials Science
Duke University
144 Hudson Hall, Box 90300
Durham, NC 27708

**Date:** June 6, 2017

## Broad Objectives

QUEST is a SciDAC Institute comprising Sandia National Laboratories, Los Alamos National Laboratory, University of Southern California, Massachusetts Institute of Technology, 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 Duke effort focuses on the development of algorithms and utility software for non-intrusive sparse UQ representations, and on participation in the organization of annual workshops and tutorials to disseminate UQ tools to the community, and to gather input in order to adapt approaches to the needs of SciDAC customers.

## Accomplishments

### UQTk

DU contributed to the October 2013 release of version 2.0 of UQTk. Version 2.0 includes capabilities for intrusive and non-intrusive propagation of uncertainty with Polynomial Chaos expansions, both in C++ and Matlab, as well as a C++ Markov chain Monte Carlo library for Bayesian inference, a C++ Bayesian Compressive Sensing (BCS) library, and a C++ library for computing Karhunen-Loève (KL) expansions from stochastic process samples.

### Multiscale Stochastic Preconditioners

We have developed a preconditioned Bayesian regression method that enables sparse representations of noisy outputs of ODE systems that exhibit large variability with random input data. The approach is based on the definition of appropriate multiscale transformations of state variables coupled with a Bayesian regression formalism. This enables efficient and robust recovery of both the transient dynamics and the corresponding noise levels. We have demonstrated the implementation of the present approach to stochastic chemical systems with uncertain reaction rates. Numerical experiments show that Bayesian preconditioning algorithms can simultaneously accommodate large noise levels and large variability with uncertain parameters, and that robust estimates can be obtained with a small number of realizations of the stochastic simulator.

### Gradient-Based Approach to Inverse Problems

We have also explored the possibility of using gradient based optimization algorithms in order to determine posterior distributions of uncertain parameters. Specifically, we have developed an approach that exploits the adjoint and the Hessian of sparse PC representations of quantities of interest with line search optimization algorithms. The inference problem is then recast in the context of a variational parameter estimation problem where the gradients of the surrogate are used to minimize the mismatch between observations and model predictions. Implementation of this methodology was demonstrated using extreme-scale simulations of the oceanic circulation in the Pacific under typhoon conditions. Results were validated by comparing the resulting predictions of optimal parameters and their local distributions with detailed estimates obtained using a Bayesian inference approach where the full posterior distribution was constructed using an adaptive MCMC technique. Experiences have shown that the adjoint/Hessian based algorithm is very efficient, and that is yields accurate prediction of optimal parameters as well as suitable estimates of the width of their distributions.

### Adaptive Pseudospectral Approximation

We have developed an adaptive pseudospectral approximation algorithm that enables construction of global surrogrates expressing the dependence of QoIs on deterministic design variables and uncertain model parameters. To enable control of the resolution in the space of design variables and uncertain parameters, the adaptive pseudospectral construction was enriched with conditional Sobol indices, that guide anisotropic refinement along individual dimensions. We have compared the performance of the resulting algorithms to hierarchical constructions employing nested pseudospectral approximations. Tests have shown that whereas the nested approach enables greater control, the Sobol-enriched pseudospectral construction yields superior performance while enable suitable error control and accommodating simple termination criteria.

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### Stochastic Limit Cycles

We have developed an intrusive PC method that enables the determination of stochastic limit cycles. The method overcomes the well-known difficulties of PC representations for long time integration, which typically manifest themselves in the form of a convergence breakdown. This is accomplished by introducing a stochastic time scaling, and using this rescaling in conjunction with Newton iterations to control the phase drift between stochastic trajectories. The efficiency of the resulting scheme was demonstrated through applications to the 2D Navier-Stokes equations. In particular, the tests indicated that the stochastic limit cycle can be suitably represented with low order PC expansions.

**PC Analysis of Noisy Uncertain Systems**

We have developed a class of PC algorithms for the analysis of stochastic differential equations driven by additive or multiplicative Wiener noise. For this setting, the algorithms rely on a Galerkin formalism that naturally leads to the definition of a hierarchy of stochastic differential equations governing the evolution of the PC modes. Under the mild assumption that the Wiener and uncertain parameters can be treated as independent random variables, the algorithms enable us to perform an orthogonal decomposition of the process variance, and consequently decompose the latter into contributions arising from the uncertainty in parameters, the stochastic forcing, and a coupled term. Insights resulting from this decomposition were gained through various implementations to simplified models problems, as well as complex systems involving unstable fixed points.

We have also developed a mathematical and computational approach that enables quantification of the inherent sources stochasticity and of the corresponding sensitivities in stochastic simulation algorithms (SSAs). The approach is based on reformulating SSAs as being generated by standardized Poisson processes. This reformulation affords a straightforward identification of individual realizations, and consequently a quantitative characterization of the inherent sources of stochasticity in the system. By relying on the Sobol-Hoeffding decomposition, the reformulation also enables us to perform an orthogonal decomposition of the solution variance. Thus, by judicioulsy exploiting the inherent stochasticity of the system, one is able to quantify the variance-based sensitivites associated with individual reaction channels, as well as the impact of channel interactions.

**Dimensionality Reduction for Bayesian Inference of Random Fields**

We have explored a new dimension reduction framework suitable for Bayesian inference based on prior Gaussian fields with uncertainty in the covariance function hyper-parameters. This traditionally achieved using the KL expansion of a prior Gaussian process assuming covariance function with fixed hyper-parameters, despite the fact that these are uncertain in nature. The posterior distribution of the KL coordinates is then inferred using available observations. The resulting inferred field is therefore dependent on the assumed hyper-parameters. Alternatively, we have developed a scheme to efficiently estimate both the field and covariance hyper-parameters using Bayesian inference. To this end, a generalized KL expansion is derived using coordinate transformations to account for the dependence with respect to the covariance hyper-parameters. PC expansions are then employed for the acceleration of the Bayesian inference using similar coordinate transformations, enabling us to avoid expanding explicitly the solution dependence on the uncertain hyper-parameters. We demonstrated the feasibility of the proposed method on a transient diffusion equation by inferring spatially-varying log-diffusivity fields from noisy data. The inferred profiles were found closer to the true profiles when including the uncertainty in the hyper-parameters in the inference formulation.

**Large-scale demonstrations**

In order to assess the performance of QUEST UQ tools, we have ported our OGCM (HYCOM-based) simulatations onto NERSC platforms, and have launched a simulation campaign focusing on combined impact of initial condition uncertainty (expressed in terms of truncated KL expansion) and variability in wind forcing (expressed in terms of space-time EOFs) on the oceanic circulation in the Gulf of Mexico. We are currently applying a combination of QUEST algorithms for the purpose of generating surrogates of QoIs obtained from ocean general circulation model (OGCM) computations. Specifically, we are focusing on the response of the circulation in the Gulf of Mexico (GOM) to uncertainties in initial conditions and wind forcing. The challenges that arise concern the high computational cost of highly resolved simulations, and the fact for extreme values of random inputs the system may evolve outside the range of validity of some of its parameterizations. The latter situation presents itself as a case of missing data. To address this difficulty, we used a combination of adaptive quadrature concepts and sparse regression techniques. We also explored the possibility extending adaptive refinement techniques to the situations where the QoIs represent field quantities.

## Publications

### Journal Publications


1. M. Vohra, X. Huan, T. Weihs, O. Knio (2017) "Design Analysis for Optimal Calibration of Diffusivity in Reactive Multilayers," *Combustion Theory and Modelling*, in press.

2. M. Navarro Jimenez, O.P. Le Maître, O.M. Knio (2016) "Global Sensitivity Analysis in Stochastic Simulators of Uncertain Reaction Networks," *J. Chem. Phys.* **145**, 244106.

3. A.A. Contreras, O.P. Le Maître, W. Aquino, O.M. Knio (2016) "Multi-Model Polynomial Chaos Surrogate Dictionary for Bayesian Inference in Elasticity Problems," *Probabilistic Engineering Mechanics* **46**, 107-119.

4. I. Sraj, S.E. Zedler, O.M. Knio, C.S. Jackson, I. Hoteit, (2016) "Polynomial Chaos-based Bayesian Inference of K-Profile Parametrization in a General Circulation Model of the Tropical Pacific," *Mon. Wea. Rev.* **144**, 4621-4640.

5. G. Li, M. Iskandarani, M. Le Henaff, O.P. Le Maître, O.M. Knio (2016) "Quantifying initial and wind forcing uncertainties in the Gulf of Mexico," *Comput. Geosci.* **20**, 1133-1153.

6. M. Iskandarani, M. Le Henaff, W. Thacker, A. Srinivasan, O. Knio (2016) "Quantifying uncertainty in Gulf of Mexico forecasts stemming from uncertain initial conditions," *Journal of Geophysical Research: Oceans* **121**, 4819-4832.

7. M. Iskandarani, S. Wang, A. Srinivasan, W.C. Thacker, J. Winokur, O. Knio (2016) "An overview of uncertainty quantification techniques with application to oceanic and oil-spill simulations," *Journal of Geophysical Research: Oceans* **121**, 2789-2808.

8. S. Wang, M. Iskandarani, A. Srinivasan , W.C. Thacker, J. Winokur, O. Knio (2016) "Propagation of uncertainty and sensitivity analysis in an integral oil-gas plume model," *Journal of Geophysical Research: Oceans* **121**, 3488-3501.

9. R. Gonçalves, M. Iskandarani, A. Srinivasan, W.C. Thacker, E. Chassignet, O. Knio (2016) "Quantifying Uncertainty In An Oil-Fate Model Using a Polynomial Chaos Surrogate," *Journal of Geophysical Research: Oceans* **121**, 2058-2077.

10. J. Winokur, D. Kim, F. Bisetti, O.P. Le Maître, O.M. Knio (2016) "Sparse Pseudo Spectral Projection Methods with Directional Adaptation for Uncertainty Quantification," *J. Scientific Computing* **68**, 596-623.

11. I. Sraj, O.P. Le Maître, O.M Knio, I. Hoteit (2016) "Coordinates Transformation and Polynomial Chaos for the Bayesian Inference of a Gaussian Process with Parametrized Prior Covariance Function," *Comput. Methods Appl. Mech. Engrg.* **298**, 205–228.

12. O.P. Le Maître, O.M. Knio (2015) "PC Analysis of Stochastic Differential Equations driven by Wiener noise," *Reliability Engineering and System Safety* **135**, 107-124.

13. O.P. Le Maître, O.M. Knio, A. Moraes (2015) "Variance Decomposition in Stochastic Simulators," *J. Chem. Phys.* **142**, 244115.

14. M. Vohra, J. Winokur, K.R. Overdeep, P. Marcello,T.P. Weihs, O.M. Knio (2014) "Development of a Reduced Model of Formation Reactions in Zr-Al Nanolaminates," *J. Appl. Phys.* **116**, 233501.

15. P. Sochala, O. Le Maître (2014) "Polynomial Chaos Expansions for Subsurface Flows with Uncertain Parameters" *Advances in Water Resources*, **62**-A, 139-154.

16. L. Tamellini, O. Le Maître and A. Nouy (2014) "Model reduction based on Proper Generalized Decomposition for the stochastic steady incompressible Navier-Stokes equations," *SIAM J. Sci. Comput.* **36**, A1089–A1117.

17. A. Alexanderian, F. Rizzi, M. Rathinam, O.P. Le Maître & O.M. Knio (2014) "Preconditioned Bayesian Regression for Stochastic Chemical Kinetics," *Journal of Scientific Computing* **58**, 592-626.

18. I. Sraj, M. Iskandarani, C. Thacker, A. Srinivasan, O.M. Knio (2014) "Drag Parameter Estimation Using Gradients and Hessian from a Polynomial Chaos Model Surrogate," *Monthly Weather Review* **142**, 933-941.

19. J. Winokur, P. Conrad, I. Sraj, O.M. Knio, A. Srinivasan, W.C. Thacker, Y. Marzouk & Mohamed Iskandarani (2013) "A Priori Testing of Sparse Adaptive Polynomial Chaos Expansions Using an Ocean General Circulation Model Database", *Comput. Geosci.* **17**, 899-911.

20. I. Sraj, M. Iskandarani, A. Srinivasan, W.C. Thacker, J. Winokur, A. Alexanderian, C.-Y. Lee, S.S. Chen & O.M. Knio (2013) "Bayesian Inference of Dependence of Drag Coefficient on Wind Speed using AXBT data from Typhoon Fanapi," *Mon. Wea. Rev.* 141:2347-2367.

**Conference Presentations**

1. P. Mycek, A. Contreras, O.P. Le Maître, K. Sargsyan, F. Rizzi, K. Morris, C. Safta, B.J. Debusschere, O.M. Knio (2016) "A Resilient Domain Decomposition Approach for Extreme Scale UQ Computation," presented at 17th SIAM Conference on Parallel Processing for Scientific Computing, Paris, France, April 12-15.

2. O.M. Knio (2016) "Surrogate based approaches to parameter inference in ocean models," presented at Workshop on Advances in Uncertainty Quantification Methods, Algorithms and Applications, KAUST, January 5-10.

3. O. Knio (2015) "Application of UQ Principles to Calibration, Sensitivity, and Experimental Design," presented at IMA Hot Topics Workshop on Uncertainty Quantification in Materials Modeling, Purdue University, West Lafayette, IN, July 28-31.(**invited**)

4. O. Knio (2015) "Application of spectral methods to forward uncertainty propagation, sensitvity analysis, and inverse design," presented at UMRIDA Workshop, TU Delft, April 15–16. (**invited**)

5. O. Knio (2014) "Bayesian approaches to model calibration in ocean general circulation models," presented at Workshop on Atmospheric and Ocean Modeling, American University of Beirut, July 30 – August 1. (**invited**)

6. M. Iskandarani, M. Le Henaff, W.C. Thacker, O.M. Knio, A. Srinivasan (2014) "Quantifying Initial Conditions Uncertainty in Gulf of Mexico Circulation Forecasts Using a Non-Intrusive Polynomial Chaos Method," presented at SIAM UQ 14, Savannah, GA, March 31–April 3.

7. J. Winokur, O.M. Knio (2014) "Hierarchical Sparse Adaptive Sampling in High Dimension," presented at SIAM UQ 14, Savannah, GA, March 31–April 3.

8. O.M. Knio (2013) "Role of Uncertainty Quantification in Questions of Sustainability Research," presented at Workshop on Theory and Knowledge for Sustainability, Santa Fe Institute, Santa Fe, NM, October 22-24. (**invited**)

9. O.M. Knio (2013) "Surrogate based inference in ocean general circulation models," presented at Oxford Conference on Challenges in Applied Mathematics, Oxford, UK, July 1-5. (**invited**)

10. O.P. Le Maître, O.M. Knio (2013) "Polynomial Chaos Expansions for the Approximation of Uncertain Stochastic Model Solutions," presented at Workshop on Numerical Methods for Uncertainty Quantification, University of Bonn, May 13-17.

11. F. Rizzi, M. El Morsli, F. Bisetti, O.M. Knio (2013) "Quantifying Uncertainty of Ion Chemistry in Premixed Methane-air Flames," presented at SIAM Fourteenth International Conference on Numerical Combustion, San Antonio, TX, April 8 - 10.

12. O.M. Knio (2013) “Surrogate Based Approaches to Parameter Inference in Ocean General Circulation Models,” presented at IMA Annual Program Year Workshop Stochastic Modeling of the Oceans and Atmosphere, Minneapolis, MN, March 11-15. (**invited**)

13. I. Sraj, M. Iskandarani, A. Srinivasan, C. Thacker, J. Winokur, A. Alexanderian, C.-Y. Lee, S. Chen. O.M. Knio (2013) “Bayesian Inference of Wind Drag using AXBT Data,” presented at SIAM Conference on Computational Science and Engineering, Boston, MA, February 25 - March 1.

14. O.P. Le Maître, A. Alexanderian, F. Rizzi, M. Rathinam, O.M. Knio (2013) “Preconditioned Bayesian Regression for Stochastic Chemical Kinetics ,” presented at SIAM Conference on Computational Science and Engineering, Boston, MA, February 25 - March 1.

15. P. Conrad, J. Winokur, I. Sraj, A. Alexanderian, M. Iskandarani, A. Srinivasan, Y. Marzouk, O. Knio (2012) “Sparse Adaptive Polynomial Chaos Representations for Ocean General Circulation Models,” presented at 9th AIMS Conference, Orlando, FL, July 1-5, 2012. (**invited**)

16. J. Winokur, P. Conrad, I. Sraj, A. Alexanderian, M. Iskandarani, A. Srinivasan, Y. Marzouk, O.M. Knio (2012) “A Priori Testing of Adaptive Sampling and Sparse PC Representations for Ocean General Circulation Models,” presented at 2012 SIAM International Conference on Data Mining, Anaheim, CA, April 26-28, 2012. (**invited**)

17. O.M. Knio (2012) “Polynomial Chaos Approaches to Multiscale and Data Intensive Computations,” presented at SIAM Conference on Uncertainty Quantification, Raleigh, NC, April 2-5, 2012. (**plenary**)

18. J. Winokur, A. Alexanderian, I. Sraj, M. Iskandarani, A. Srinivasan, C. Thacker, O. Knio (2011) “Quantifying Parametric Uncertainty in Ocean General Circulation Models: A Sparse Quadrature Approach,” presented at the DFD11 Meeting of the American Physical Society.