FINAL REPORT

- PROJECT TITLE: MATHEMATICAL AND COMPUTATIONAL TOOLS FOR PREDICTIVE SIMULATION OF COMPLEX COUPLED SYSTEMS UNDER UNCERTAINTY
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- Distribution Limitations: None.

Executive Summary

The research completed under this project contributes critical capabilities and understanding to the general area of uncertainty quantification and in particular as it pertains to multiscale and multiphysics problems. In particular, we have developed capabilities that successfully tackle the curse of dimensionality in these problems by taking advantage of the mathematical structure of the problems, without relaxing constraints on accuracy and rigour. This is paramount for relying, credibly, on simulations from flagship computational platforms for critical decisions. In addition, we have developed a new path of exploration that permits the adaptation of models and their data to quantities of interest. An inverse problem is thus no longer only associated with a governing equation and measurements. The ultimate quantity of interest in the simulations is critically relevant to the formulation of the inverse problem.

The concepts and algorithms developed under the present effort substantially increase the comfort zone within which decision makers can rely, with certifiable confidence, on computer simulations of complex systems.

Comparison of Actual Accomplishments with Goals and Objectives

The actual accomplishments extended the initial goals and objectives by obtaining results and algorithms that are valid across a much wider class of applications than originally anticipated. Two specific extensions are worth noting: 1) Embedded quadratures were derived to enable the segregation of uncertainties in multiphysics problems by allowing each sub-problem to be solved within a stochastic dimension controlled by its own uncertainty. The resulting embedded quadratures permit the evaluation of integrals of composite functions with respect to the measure of the composition, instead of the original measure. Multiscale integrals, for instance, are evaluated with respect to the coarse scale measure while retaining information from the subscale. 2) Adapting the stochastic expansion bases to a quantity of interest is a generic approach with implications across stochastic analysis, and not merely to the class of problems initially considered in this project.

Summary of Project Activities

The project activities progressed along three main lines : 1) linear solvers for equations arising in stochastic galerkin projections, 2) model adaptation for stochastic multiphysics problems, and 3) bases adaptations for specific quantities of interest (QoI). These are detailed in the next three subsections. Except for the third approach, the other two were part of our proposed tasks. The third item emerged as we gained experience with the procedures we were developing and developed a better appreciation to the challenges and mathematical structure.

Linear Solvers

In the area of linear solvers, we developed procedures that took advantage of a hierarchical structure of the matrices involved, thus permitting us to develop a recursive Schur decomposition according to which we only had to solve a set of linear equations along the block diagonals of the stochastic galerkin matrix. The structure of these matrices is inherited from the orthogonality property of Hermite (or any other system of orthogonal) polynomials. Figure (1) depicts the relevant structure. In some situations, the matrix has a denser non-zero structure. In those cases, a preconditioner built from this same zero structure still performs quite well. Alternatively, in the case of denser matrices, we also developed a procedure that truncates the matrix-vector products in an iterative process to a sub-band in the global matrix. This sub-band is identified based on the norm of the block matrices appearing in the global matrix. Figure (2) shows the norm of these sub-matrices, within the global matrix.

Figure 1: Block structure of the global stochastic galerkin matrix highlighting the block structure used in building the recursive Schur iterative scheme.

Figure 2: Color-coded rendition of the block structured matrix depicting the norm of the submatrices.

Stochastic Multiphysics

One of the challenges in multiphysics problems pertains to the deconvolution of variables that are specific to each of the individual physics problems. To address this challenge, we developed a Karhunen-Loeve expansion for the output of one physical model with random variables dependent on the sources of uncertainty of that particular model, and whose coefficients (usually deterministic) are functions of the random variables describing the other physics. This has permitted us to analyze the coupled problem using separate model problems, each described within its own uncertainty framework. Thus instead of analyzing the coupled problem within an $s_1 + s_2$ dimensional setting, we analyze it within two problems, one of dimension s_1 and the other of dimension s_2 . The computational savings are obvious.

In addition, we developed a procedure for the very efficient evaluation of integrals of composite functions. Where the original dependence is in a high dimensional space, but the function we care about is a composite mapping into a much lower dimensional space. This is

typical in a multi-scale setting. Figure (3) shows quadrature points with respect to the initial measure and the quadrature points in the composite measure to evaluate within the same accuracy a typical integral appearing in a multiscale calculation. The number of function evaluations in the new measure is clearly a fraction of the evaluations in the original measure.

Figure 3: Plots showing the quadrature points overlaid on a two-dimensional contour plot of the joint density function of two random variables. Left: quadrature points in standard approach; Right: quadrature points in adapted embedded approach.

Basis Adaptation to QoI

We developed a basis adaptation scheme that permits us to adapt the basis in the polynomial chaos expansion to scalar quantities of interest. The resulting basis is typically either one-dimensional or consisting of a sequence of one-dimensional bases. The number of bases in this approximation is typically linear with the dimension of the stochastic approximation, which is in sharp contrast with the standard multi-dimensional bases which grows exponentially with that dimension. Figure (4) shows approximations obtained using a full multivariate expansion (10 dimensional) together with approximations obtained using the best KL dimension, and two approximation schemes developed in this research.

Products Developed under Award

The products detailed in the following subsection were developed under this award.

Refereed Journal Papers

1. Sousedik, B. and Ghanem, R., “Truncated hierarchical preconditioning for the stochastic Galerkin FEM,” submitted to *International Journal on Uncertainty Quantification*.
2. Arnst, M., Ghanem, R., Phipps, E., and Red-Horse, J., “Reduced chaos expansions with random coefficients in reduced-dimensional stochastic modeling of coupled problems,” submitted to *International Journal for Numerical Methods in Engineering*.

Figure 4: The probability density function (right) and its tail (left) for the displacement at one point in an elastic medium subjected to static loading. The figures show approximations obtained using a full multivariate expansion (10 dimensional) together with approximations obtained using the best KL dimension, and two approximation schemes developed in this research.

3. Sousedik, B., Ghanem, R., and Phipps, E., “Hierarchical Schur complement preconditioner for the stochastic Galerkin finite element methods,” in press, *Numerical Linear Algebra with Applications*, 2013.
4. Arnst, M., Ghanem, R., Phipps, E., and Red-Horse, J., “Measure transformation and efficient quadrature in reduced-dimensional stochastic modeling of coupled problems,” *International Journal for Numerical Methods in Engineering*, Vol. 92, No. 12, pp. 1044-1080, 2012.
5. Arnst, M., Ghanem, R., Phipps, E., and Red-Horse, J., “Dimension reduction in stochastic modeling of coupled problems,” *International Journal for Numerical Methods in Engineering*, Vol. 92, No. 11, pp. 940-968, 2012.
6. Arnst, M. and Ghanem, R., “A variational-inequality approach to stochastic boundary value problems with inequality constraints and its application to contact and elastoplasticity,” *International Journal for Numerical Methods in Engineering*, Vol. 89, No. 13, pp. 1665-1690, 2012.
7. Arnst, M., Ghanem, R. and Masri, S., “Maximum entropy approach to the identification of stochastic reduced-order models of nonlinear dynamical systems,” *The Aeronautical Journal*, Vol. 114, No. 1160, pp. 637-650, 2010.
8. Arnst M., Ghanem R., Soize C., “Identification of Bayesian posteriors for coefficients of

chaos expansions,” *Journal of Computational Physics*, Vol. 229, No. 9, pp. 3134-3154, 2010.

9. Arnst, M. and Ghanem, R., “Probabilistic electromechanical modeling of nanostructures with random geometry” *Journal of Computational and Theoretical Nanoscience*, Vol. 6, No. 10, pp. 2256-2272, 2009.

Conference Presentations

1. Tipireddy, R. and Ghanem, R., “Stochastic reduced models,” *SIAM CS&E Conference*, Boston, MA, February 25-March 1, 2013.
2. 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.
3. 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.
4. 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.
5. Ghanem, R. and Tipireddy, R., “Stochastic basis reduction via QoI adaptation,” *SIAM First Conference on Uncertainty Quantification*, Raleigh, NC, April 2-5, 2012.
6. Arnst, M. and Ghanem, R., “Stochastic analysis of coupled dynamical systems,” *ASCE Engineering Mechanics Institute Conference*, Los Angeles, CA, Aug 8-11, 2010.
7. Phipps, E., Eldred, M., Ghanem, R., Pawlowski, R., Red-Horse, J., Schmidt, R., and Stripling, H., “Stochastic Dimension Reduction for Network Coupled Systems,” *AN10: SIAM Annual Meeting*, Pittsburgh, PA, June 12-16, 2010.
8. Ghanem, R. and Arnst, M., “An assessment of stochastic model reduction methods,” *European Conference on Computational Mechanics*, Paris, France, May 16-21, 2010.
9. Arnst, M. and Ghanem, R., “Formulation and solution of stochastic variational inequalities describing inelastic material behavior and contact/impact,” *10th US National Congress on Computational Mechanics*, Columbus, OH, July 16-19, 2009.

Networks or Collaborations Fostered

The PI is currently involved as co-PI in QUEST, a SciDAC Institute on Uncertainty Quantification. This involvement is the direct product of this award which facilitated the PI’s collaboration with colleagues at Sandia, and with other colleagues supported through ASCR and who eventually formed the QUEST team (eg. colleagues at Los Alamos, Sandia, MIT Duke, UT-Austin).

Computer Modeling

The models developed under this award were integrated into Stokhos by our Sandia Collaborator and co-PI, Dr. Eric Phipps. These developments fall into three categories, namely 1) solvers for stochastic Galerkin equations, 2) adapted bases in stochastic projections, and 3) reduced models for stochastic multiphysics problems. The software tools and computational capabilities are being expanded and developed at Sandia. Students and postdocs involved with this project did spend time at Sandia-Albuquerque working closely with Dr. Phipps.