Final Report: DE-FG02-95ER25239 Spectral Representations of Uncertainty: Algorithms and Applications

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1 Objectives of this project

- Develop a general algorithmic framework for stochastic ordinary and partial differential equations.
- Set polynomial chaos method and its generalization on firm theoretical ground.
- Quantify uncertainty in large-scale simulations involving CFD, MHD and microflows.
- The overall goal of this project was to provide DOE with an algorithmic capability that is more accurate and three to five orders of magnitude more efficient than the Monte Carlo simulation.

2 Summary of Main Results

In the previous grant we developed a new approach for solving stochastic differential equations corresponding to general stochastic inputs. Specifically, we developed a generalized polynomial chaos (GPC) method for stochastic ODEs as well as for stochastic advection, diffusion and Navier-Stokes equations.

Here we review briefly GPC. This approach extends the original ideas of Norbert Wiener on Hermite expansions (suitable for Brownian motion) to other more effective polynomial

functional bases. The new broader basis is derived from the *generalized hypergeometric series* that lead to many different orthogonal polynomials, the so-called *Askey family*.

The chaos expansion is essentially a representation of a function $f \in L_2(\Omega)$ where Ω is a properly defined probability space. We denote by $\{\Phi_k\}_{k=0}^{\infty}$ the orthogonal polynomials from the Askey scheme, which form an orthogonal basis in L_2 . A general second-order random process $X(\omega)$ can be represented in the form

$$X(\omega) = \sum_{j=0}^{\infty} a_j \Phi_j(\xi(\omega)). \quad (1)$$

In the original polynomial chaos, $\{\Phi_n\}$ are the *Hermite* polynomials and ξ are the *Gaussian* random variables. In the Askey-chaos expansion, the orthogonal polynomials $\{\Phi_n\}$ are not restricted to Hermite polynomials; instead, they are determined by the weighting function of the corresponding random variables ξ , which are not necessarily Gaussian variables. For example, for a uniform distribution the Legendre polynomial functionals are the best representation whereas for a Poisson distribution the Charlier polynomial functionals form the optimum basis.

In the following we review the main results we have obtained for prototype differential equations and applications.

2.1 Ordinary Differential Equations

1. D. Xiu and G.E. Karniadakis, "The Wiener-Askey Polynomial Chaos for stochastic differential equations", SIAM Journal of Scientific Computing, vol 24, no. 2, pp. 619-644, 2002.

Here we consider a first-order ODE with the reaction constant as an uncertain process, i.e. a random variable that may vary in time. We have developed the first algorithms for the Wiener-Askey chaos using this ODE as a model and have demonstrated their resolution properties. Specifically, it was shown that, for certain type of uncertainty input, the properly chosen generalized polynomial chaos expansion converges *exponentially* fast. Although the Hermite-chaos shows exponential convergence for Gaussian input, it does *not* do so for other inputs. In particular, for a *Gamma* random input, the proper generalized polynomial chaos, the Laguerre-chaos, converges exponentially fast whereas for the Hermite-chaos the convergence rate is severely deteriorated. Other issues such as how to represent an arbitrary random input by a chosen basis, were presented.

2.2 Diffusion Equation

1. D. Xiu and G.E. Karniadakis, "Modeling uncertainty in steady state diffusion problems via generalized polynomial chaos", *Comput. Methods Appl. Mech. Engrg.*, vol. 191, pp. 4927-4948, 2002.
2. D. Xiu and G.E. Karniadakis, "Modeling Uncertainty of Elliptic Partial Differential Equations via Generalized Polynomial Chaos", *Proceedings of the 5th ASCE Engineering Mechanics Division Conference*, Columbia University, New York City, June 2002.
3. X. Wan, D. Xiu and G.E. Karniadakis, "Modeling uncertainty in three-dimensional heat transfer problems", *Heat Transfer Conference*, Lisbon, Portugal, March 24-26, 2004.

In the above published papers, the steady state diffusion problems subject to stochastic diffusivity, forcing and boundary conditions, was solved by the generalized polynomial chaos expansion. A block Gauss-Seidel iteration algorithm was designed to solve the coupled (in random space) set of equations efficiently. Exponential convergence rate was demonstrated for one-dimensional model problem with different types of uncertain inputs. In two-dimensions, a more realistic correlation model expressed by the Bessel correlation function was investigated and employed. A new algorithm to represent stochastic processes as input to the three-dimensional code has also been formulated.

We have shown theoretically that the discrete Wiener-Hermite system for diffusion leads to an ill-posed problem. This implies that for any value of standard deviation, however small, the expansion will diverge as we increase the order of the polynomial chaos. In contrast, the Jacobi-chaos (appropriate for general Beta distributions) is always well-posed as long as the magnitude of standard deviation is less than the mean value. This may explain some of the difficulties reported occasionally in the literature regarding the classical Hermite expansions.

2.3 Advection and Advection-Diffusion Equations

1. M. Jardak, C.-H. Su and G.E. Karniadakis, "Spectral Polynomial Chaos solutions of the stochastic advection equation", *J. Sci. Comp.*, vol. 17, pp. 319-338, 2002.
2. D. Xiu and G.E. Karniadakis, "Uncertainty Modeling of Burgers' Equation by Generalized Polynomial Chaos", *Proceedings of the 4th International Conference on Computational Stochastic Mechanics*, Corfu, Greece, June 2002.

3. D. Xiu and G.E. Karniadakis, "Supersensitivity due to uncertain boundary conditions", *Int. J. Num. Meth. Eng.*, vol. 61, pp. 2114-2138, 2004.
4. X. Wan, D. Xiu and G.E. Karniadakis, "Stochastic solutions for the two-dimensional advection-diffusion equation", *SIAM J. Sci. Comput.*, vol. 26(2), pp. 578-590, 2004.

Here we developed a new algorithm based on Wiener-Hermite functionals combined with Fourier collocation to solve the linearized advection equation with stochastic transport velocity. We formulated different strategies of representing the stochastic input, and demonstrated that this approach is orders of magnitude more efficient than Monte Carlo simulations for comparable accuracy. We also derived exact analytical stochastic solutions to serve as benchmarks in future work.

In addition, we considered the issue of uncertainty in the boundary conditions and use the Burgers's equations as a model problem. We demonstrated supersensitivity of the nonlinear system by showing that even infinitesimally small perturbations on the boundaries could lead to order one changes in the mean stochastic response.

2.4 Navier-Stokes Equations

1. D. Xiu and G.E. Karniadakis, "Modeling uncertainty in flow simulations via Generalized Polynomial Chaos", *J. Comp. Phys.*, vol. 187, p. 137, 2003.
2. D. Lucor, D. Xiu, C.-H. Su and G.E. Karniadakis, "Predictability and uncertainty in CFD", *Int. J. Num. Meth. Fluids*, vol. 43(5), pp. 485-505, 2003.

Here the generalized polynomial chaos was applied to the uncertainty modeling in incompressible Navier-Stokes equations. The expansion algorithm, coupled with a high-order time-splitting scheme, was discussed. The spatial discretization is the spectral/*hp* element method. A microfluidics problem, i.e. channel flow with random boundary conditions, was solved. The chaos expansion results were validated against exact solutions (when available) and solutions of Monte Carlo simulations. Good agreement was obtained between the solutions of chaos expansions and those of Monte Carlo with more than 100,000 realizations. In this case, the chaos expansion is at least $2 \sim 3$ orders faster. As a more complicated problem, the flow past a circular cylinder with upstream noise was solved. We investigated the effect of upstream perturbation on the transition at $Re = 40 \sim 50$, as well as the stochastic nature of the flow at moderate Reynolds number, e.g. $Re = 100$.

In addition, the general aspect of the stochastic modeling of CFD-related problems via polynomial chaos was presented in the invited paper in IJNMF (2003). Also, a flow-structure

interaction problem was studied in detail, examining for example the uncertainty in the vortex structure, development of the probability distribution of pressure on the cylinder, and the vortex-induced vibration of the cylinder. Open issues were addressed, specifically some difficulties associated with the Hermite-chaos expansion, and its slow convergence in certain cases.

3 Invited Presentations

- AFOSR Uncertainty Workshop, Albuquerque, March 2002.
- Mission Computing Conference (NASA/DOE/DOD), Keynote Speaker, February 2003.
- Northwestern University, Applied Mathematics seminar, March 2003.
- WPI, Mechanical Engineering seminar, March 2003.
- Computational Science and Engineering Symposium at University of Illinois, Urbana-Champaign, Keynote Speaker, April 2003.
- Northwestern University, Mechanical Engineering seminar, September 2003.
- MIT High Performance Distinguished Speakers series, October 2003.
- Bluff Body and VIV Conference, invited speaker, December 2003.
- Institute for Advanced Studies, Princeton, December 2003 (Dongbin Xiu).
- Los Alamos Workshop, December 2003 (Dongbin Xiu).
- Los Alamos National Laboratory, January 2004.
- International Symposium on Mechanical Systems Innovation, Keynote Speaker, University of Tokyo, March 2004.
- Department of Mathematics, Tufts University, December 2004.

4 Personnel

The following people were supported by this grant:

- G.E. Karniadakis, PI.
- Dongbin Xiu, PhD student (ODEs/PDEs).
- Didier Lucor, PhD student (Navier-Stokes).
- Mike Kirby, PhD student (spectral elements).
- Steven Dong, Postdoc (parallel computing).

We note that all three PhD students supported by this grant (Xiu, Lucor and Kirby) have now tenure-track Professorships at Purdue University, University of Paris VI, and University of Utah, respectively.