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1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE		3. DATES COVERED (From - To)
07/31/2006	Final		1 March 2003- 30 June 2006

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Stochastic Spectral/ HP Element Methods for CFD and MHD Simulations	
	5b. GRANT NUMBER
	F49620-03-1-0218
	5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)	5d. PROJECT NUMBER
George Karniadakis	
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
Brown University Division of applied Mathematics Providence, RI 02912	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10 SPONSOR/MONITOR'S ACRONYM(S)
Air Force Office of Scientific Research 4015 Wilson Blvd Mail Room 713 Arlington, VA 22203	AFRL-SR-AR-TR-06-0427

Dr Spogren

12. DISTRIBUTION/AVAILABILITY STATEMENT

Distribution A; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

Multi-Element Polynomial Chaos: Generalized polynomial chaos (gPC) or Wiener-Askey expansions is a method developed by the PI and his students, see [1]. This method is similar to spectral techniques - but in high-dimensions - so both Galerkin and collocation projections can be employed to produce the algebraic equations from the partial di®erential equations.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
U	U	U	UU		19b. TELEPHONE NUMBER (Include area code)

STOCHASTIC SPECTRAL/*HP* ELEMENT METHODS FOR CFD AND MHD SIMULATIONS

AFOSR GRANT NUMBER: F49620-03-1-0218

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Abstract

We have developed a new method to quantify uncertainties associated with boundary and initial conditions, transport properties, and geometry in fluid and plasma flow problems of interest to AFOSR. It is based on the pioneering ideas of Wiener on polynomial chaos for representing Gaussian processes but our method is more general and more effective for non-Gaussian processes and nonlinear problems. In the current third year of this project we have developed a multi-element version of the method whereby the random space is decomposed adaptively into small elements by tracking local values of the variance. Within each element a generalized polynomial chaos expansion is employed to represent the random processes in the spirit of discontinuous Galerkin spectral/*hp* element methods. Here we present results on adaptive refinement and convergence as well as simulations of supersonic flow past a wedge in the presence of uncertainties.

Objectives

The *long-term* objective of this work is to develop an algorithmic capability that will allow to perform **non-sterilized** flow and plasma simulations, where the input parameters and geometric domain have realistic representations. The simulation output will be denoted not by single points but by distributions that express the sensitivities of the flow to the uncertainty in the input. This will be a valuable tool for experimentalists as it will also quantify individual sensitivities to different parameters, thereby suggesting new experiments and instrumentation.

The *specific* objective is to develop stochastic simulation approaches in order to quantify the various sources of uncertainty in prototype CFD and MHD problems. Sources of uncertainty may include the boundary conditions, the physical properties, the domain, and other source and interaction terms. A new method for solving stochastic PDEs will be developed and benchmark results that verify and validate this approach will be obtained.

Accomplishments

Algorithms: Generalized polynomial chaos (gPC) or Wiener-Askey expansions is a method developed by the PI and his students, see [1], as an extension of the Wiener-Hermite poly-

nomial chaos, see [2]. The latter is more suitable for Gaussian processes whereas gPC is more effective for non-Gaussian processes. The specific aim of this project was to develop gPC for incompressible and compressible flows as well as for plasma flows. In such problems, stochasticity representing uncertainty, may be associated with boundary conditions, initial conditions, geometry or transport coefficients. In the first year of this grant, we set the foundations of gPC in modeling uncertainty for elliptic and advection-diffusion problems. In the second year, we extended the formulation to fluid and plasma flows. In particular, we have discretized the incompressible Navier-Stokes equations, compressible Euler equations, and the Korteweg-de Vries equation; the latter models noisy plasmas. Part of this work was published in the *Proceedings of the National Academy of Sciences* and was also featured on the cover of *Physical Review Letters*.

The overall procedure builds on our previous work on high-order discretizations and consists of three main components:

- A decomposition of stochastic inputs using Karhunen-Loeve expansions.

- A deterministic part based on spectral/*hp* element discretization.

- A generalized polynomial chaos representation of the stochastic solution based on the Askey family of polynomials.

In the current third year of this effort, we have addressed in depth the effectiveness and robustness of gPC in high-speed aerodynamic flows, which are typically associated with discontinuities and long-time integration. To this end, we have formulated a new method, similar to the spectral/*hp* element method, but for discretization of random space. This new method converges very fast, with the error in variance decaying as

$$\epsilon \propto N^{-2(p+1)},$$

where N is the number of random elements per dimension and p is the order of the polynomial chaos.

Specifically, we have formulated a multi-element generalized polynomial chaos (ME-gPC) method that adaptively decomposes the space of random inputs when the relative error in variance becomes greater than a threshold value. In each subdomain or random element, we then employ a gPC expansion. We have also developed a criterion to perform such a random decomposition adaptively, and demonstrate its effectiveness in long-time integration and discontinuous problems. For multi-dimensional stochastic inputs, we first test for the most sensitive dimension (or direction) and subsequently we perform the random decomposition along that dimension first, to gain efficiency.

An example in two random dimensions was presented in [3] for the Kraichnan-Orszag (K-O) model of turbulence (representing simplified turbulence interactions) with discontinuous initial conditions. In figure 1 we present the evolution of adaptive meshes for the K-O problem. It can be seen that around the discontinuity region the elements are more probable to be refined because the convergence of gPC in these elements is much slower. In figure

2 the convergence of adaptive ME-gPC is shown. Fourth-order orthogonal polynomials are employed and an adaptive criterion given in [3] is used. For comparison, the results given by fifth-order Hermite-chaos are included. It was shown in [3] that for the K-O problem, increasing the polynomial order helps very little in the convergence of gPC.
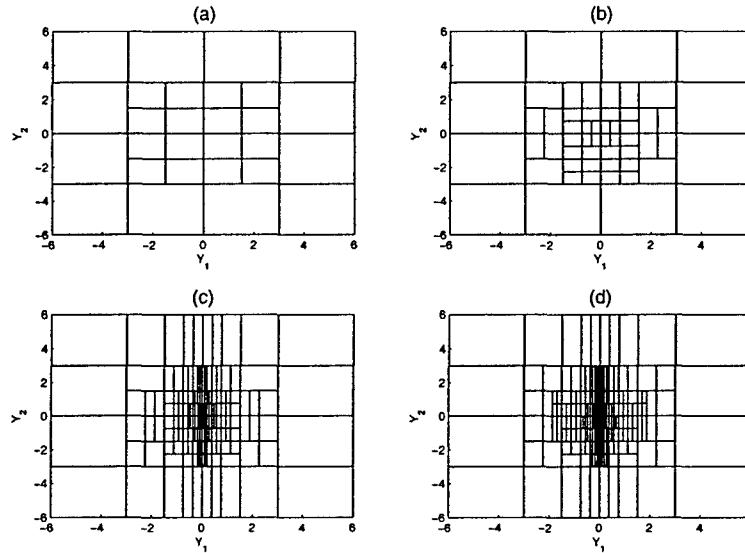

Figure 1: Two-dimensional adaptive meshes at different times for the K-O problem. (a): $t = 1$; (b): $t = 3$; (c): $t = 6$; (d): $t = 10$.

In addition to the aforementioned developments, we have also considered and resolved a very *fundamental* approximation problem, namely how to represent arbitrary probability distribution functions (PDFs) that cannot be readily represented by the Wiener-Askey polynomial chaos. ME-gPC method is based on a decomposition of the random space of stochastic inputs, and should maintain an orthogonal polynomial basis in each random element. For *uniform* random variables, such orthogonality can be inherited naturally due to the nice properties of uniform distribution. However, for an arbitrary probability measure, orthogonality will be lost due to the random decomposition. To this end, we formulated the ME-gPC method for **arbitrary probability measures**, where the orthogonality of the polynomials in each random element can be maintained by a fast numerical reconstruction. This leads to a new ME-gPC method that can achieve *h-p* convergence efficiently for *any* probability measure. Moreover, and perhaps more importantly, this will allow us to update periodically the trial basis by *tracking the PDF of the output*, instead of the input – the two being very different for strongly nonlinear problems.

Applications: We have considered three classes of applications: incompressible flows, compressible flows, and plasmas, see section on publications. In all cases we have developed *analytical solutions* based on stochastic perturbation methods in order to evaluate the accu-
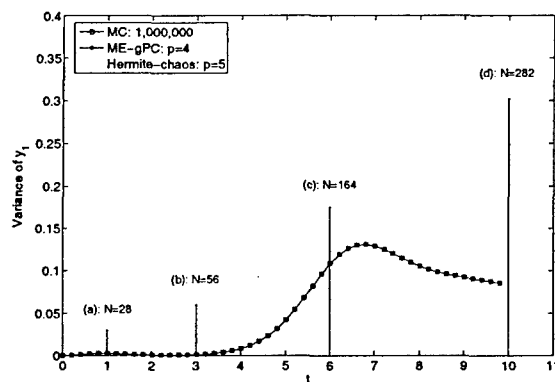
Figure 2: Convergence of adaptive ME-gPC. The indices (a)-(d) indicate the corresponding meshes in figure 1. The length of vertical straight solid lines denotes the number N of random elements.

racy of the method and also compare its efficiency with respect to Monte-Carlo simulation. In particular, for compressible flows we have simulated supersonic past a wedge – a classical problem in deterministic CFD - in the presence of random inflow disturbances or random oscillations of the wedge around its apex or even random roughness. A typical result is shown in figure 3, where we see the effect of inflow randomness on the distorted shock paths.

Open Issues
So far we have addressed one of the two main difficulties of generalized polynomial chaos, namely, the breakdown of the approximation in *long-time integration* and in the presence of *stochastic bifurcations*. The second important issue is computational complexity for *multi-dimensional* stochastic inputs; this may include problems with small correlation length. We have partially addressed this problem in preliminary work, at least for random inputs with Gaussian covariance, by developing a fast Gauss transform to deal with the many dimensions. However, we need to extend this work to non-Gaussian covariances using multipole methods for general kernels. In addition, we plan to focus on theoretical work to identify appropriate low-dimensional subspaces, and subsequently formulate the proper algorithms for reduced-order modeling. This important issue will be addressed in the next three years if this project continues. We have also obtained preliminary results on the scattering of shocks due to geometric roughness and random inflow disturbances. This is a new area of investigation and requires systematic studies as it affects directly momentum and heat transport in important flow regimes, e.g. supersonic transition.
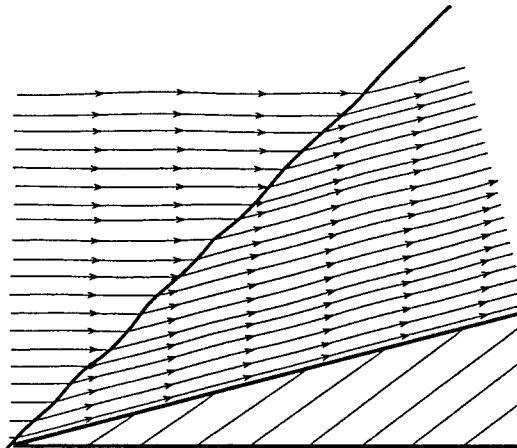
Acknowledgement/Disclaimer

Figure 3: Supersonic flow past a wedge: Perturbed shock paths induced by small time-dependent inflow perturbations. These are preliminary theoretical and numerical results in modeling the effect of random perturbations on the scattering of shocks in high-speed flows.

Research or the U.S. Government.

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[3] X. Wan and G.E. Karniadakis. An adaptive multi-element generalized polynomial chaos method for stochastic differential equations. *J. Comput. Phys.*, 209:617–642, 2005.

Personnel Supported During Duration of Grant
- Faculty: G.E. Karniadakis, Professor of Applied Mathematics.
- PhD Students: Guan Lin and Xiaoliang Wan.

Publications

1. G. Lin, C.-H. Su and G.E. Karniadakis, "The stochastic piston problem", Proceedings of National Academy of Sciences, vol. 101, pp. 15840-15845, 2004.

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6. R.M. Kirby and G.E. Karniadakis, "Selecting the Numerical Flux in Discontinuous Galerkin Methods of Diffusion Problems," Journal of Scientific Computing, Volumes 22 and 23, pp. 385-411, 2005.

Honors & Awards
- Fellow of the American Physical Society, 2004.
- Fellow of the American Society of Mechanical Engineers, 2003.

AFRL Point of Contact
Dr. Philip Beran, Principal Research Aerospace Engineer, WPAFB, OH 45433, Phone 937-255-6645. Interactions in Summer-Fall 2004.

Interactions/Transitions
The PI has been working with Prof. James Glimm (Stonybrook) to co-edit a special issue of the Journal of Computational Physics focused on uncertainty quantification. He had also interactions with Dr. Daniel Tartakovsky (Los Alamos), Prof. Triantafyllou at MIT, Prof. D. Gottlieb at Brown, Prof. A. Monti (University of South Carolina), Prof. I.G. Kevrekidis (Princeton University), and others, who have adopted the generalized Polynomial Chaos method for their scientific applications.