Uncertainty Quantification and Polynomial Chaos Techniques in Computational Fluid Dynamics

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Abstract

The quantification of uncertainty in computational fluid dynamics (CFD) predictions is both a significant challenge and an important goal. Probabilistic uncertainty quantification (UQ) methods have been used to propagate uncertainty from model inputs to outputs when input uncertainties are large and have been characterized probabilistically. Polynomial chaos (PC) methods have found increased use in probabilistic UQ over the past decade. This review describes the use of PC expansions for the representation of random variables/fields and discusses their utility for the propagation of uncertainty in computational models, focusing on CFD models. Many CFD applications are considered, including flow in porous media, incompressible and compressible flows, and thermofluid and reacting flows. The review examines each application area, focusing on the demonstrated use of PC UQ and the associated challenges. Cross-cutting challenges with time unsteadiness and long time horizons are also discussed.

1. INTRODUCTION

UQ: uncertainty quantification

CFD: computational fluid dynamics

PC: polynomial chaos

There has been increasing interest in uncertainty quantification (UQ) in computational fluid dynamics (CFD) in recent years given the development of polynomial chaos (PC) methods for the probabilistic representation of uncertainty. Key advantages of PC UQ methods include their efficiency and their utility for representing and propagating large uncertainties through complex models.

A few reviews of the applications of UQ in CFD offer different perspectives. Walters & Huyse (2002) analyzed different UQ strategies in the CFD context, including PC, sensitivity analysis, moment methods, and interval mathematics, focusing on a set of generic compressible flow model problems. Zang et al. (2002) analyzed the needs and opportunities for general uncertainty-based design methods for aerospace vehicles. Faragher (2004) reviewed UQ in CFD, touching on a number of topics, including PC, verification and validation, sensitivity analysis, and interval mathematics. Recently, Knio & Le Maître (2006) discussed the use of PC UQ in CFD, covering a number of relevant methodologies, with specific examples in incompressible flow and natural convection.

The present review surveys the use of PC UQ methods in a wide range of CFD applications. I first present an overview of UQ methods, followed by an exposition of PC theory and its utility for UQ. With this background in place, I then address the utilization of PC UQ in CFD, covering a range of application areas, including flow in porous media, as well as incompressible, thermofluid, reacting, and compressible flows. The topic of unsteady dynamics, spanning all such applications, is addressed in a focused way given its unique challenges.

2. UNCERTAINTY QUANTIFICATION

It is important at the outset to distinguish between uncertainty and numerical discretization errors. CFD code verification (Oberkampf & Blottner 1998), i.e., ensuring that the numerical solution corresponds to the underlying mathematical model, is important but is outside the present scope. Rather, this review focuses on the consequence of underlying uncertainties on model predictions. There are many sources of uncertainty in computations, including model structure, modeling assumptions, constitutive laws, model parameters, inputs, domain geometry, and initial/boundary conditions. We are concerned here with uncertainty in model parameters, which applies in general to all the above sources of uncertainty, as long as they are parameterized. In the CFD context, parameters may be global constants (e.g., a chemical rate constant in a reacting flow computation), or they may exhibit dependence on other independent variables (e.g., the spatially varying permeability of a porous medium).

The UQ problem has two intimately coupled components. The first pertains to the forward propagation of uncertainty from model parameters to model outputs, which is the focus of the present review. The second component, involving estimation of the parametric uncertainties themselves based on available data, although important, is outside the present scope and is only briefly discussed.

Numerous UQ methods have been employed in the literature. Some, such as local sensitivity analysis and moment methods (Cacuci 2003, Saltelli et al. 2000), are more suitable in the limit of small uncertainty. For large degrees of uncertainty, methods that handle uncertainty more generally using probability theory, which include PC methods, are more appropriate. Other fully probabilistic methods include global sensitivity analysis, involving statistical sampling (Saltelli et al. 2000). Sampling-based UQ methods are discussed below (albeit primarily in the PC context).

In the absence of any data or prior knowledge about parameters, except their ranges of variability, researchers have employed nonprobabilistic means of UQ (Helton et al. 2004). These include evidence theory (Oberkampf & Helton 2005) and possibility theory (de Cooman et al.

EPISTEMIC AND ALEATORIC UNCERTAINTY

Uncertainty is described as epistemic when it results from a lack of knowledge about a quantity whose true value exhibits no actual variability. Conversely, uncertainty that results from variability is termed aleatoric. Depending on the operative view of probability, parameters with epistemic uncertainty may or may not be handled in a probabilistic forward UQ context. This distinction has to do with the Bayesian versus the frequentist view of probability (Jaynes 2003). In the frequentist viewpoint, only quantities with aleatoric uncertainty, whose PDF may be constructed from their observed variability, may be modeled as random variables/fields. In contrast, there is no basis for assigning PDFs for parameters with epistemic uncertainty. This difficulty does not arise in the Bayesian viewpoint, in which probability is inherently the degree of belief in a proposition, and it does not necessarily derive from sampling or observation. In this context, parameters with epistemic uncertainty may still be assigned a PDF, as long as sufficient data and/or prior information is available to construct one. Therefore, in principle, both epistemic and aleatoric uncertainties can be handled using probability theory in the Bayesian framework.

1995), which use interval mathematics (Hansen 1992) techniques to address the propagation of uncertainty intervals. Fuzzy set theory (Cox 1999) and imprecise probability theory (Kozine 1999) have also been used in this regard. Here we presume the existence of sufficient information about model parameters to allow the assignment of probability density functions (PDFs) and/or the evaluation of their statistics, enabling probabilistic PC UQ methods (see the sidebar, Epistemic and Aleatoric Uncertainty).

Below, the basic principles of PC theory and the various methods for using PC expansions for UQ are outlined, followed by the specific applications of PC UQ in CFD.

3. POLYNOMIAL CHAOS

Consider a probability space $(\Omega, \mathfrak{S}, P)$, where Ω is a sample space, $\mathfrak{S}$ is a σ-algebra on Ω, and P is a probability measure on $(\Omega, \mathfrak{S})$. Let $\{\xi_i(\omega)\}_{i=1}^{\infty}$ be a set of independent standard Gaussian random variables (RVs) on Ω. Then we can represent any RV $X : \Omega \to \mathbb{R}$ with finite variance, i.e., $X \in L^2(\Omega)$, as

$$X(\omega) = a_0\Gamma_0 + \sum_{i_1=1}^{\infty} a_{i_1}\Gamma_1(\xi_{i_1}) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Gamma_2(\xi_{i_1}, \xi_{i_2})$$
$$+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}\Gamma_3(\xi_{i_1},\ \xi_{i_2},\ \xi_{i_3}) + \cdots, \tag{1}$$

where Γ_p is the Wiener PC of order p (Ghanem & Spanos 1991, Janson 1997, Wiener 1938) and the $a_{()} \in \mathbb{R}$. We may rewrite this polynomial chaos expansion (PCE) more compactly as

$$X(\omega) = \sum_{k=0}^{\infty} \alpha_k \Psi_k(\xi_1, \xi_2, \ldots), \tag{2}$$

where there is a one-to-one correspondence between the coefficients and functionals in Equation 1 and those in Equation 2 (Ghanem & Spanos 1991). This PC representation applies equally to random fields/processes, separating the spatiotemporal and random dependences. Thus,

$$X(\boldsymbol{x}, t, \omega) = \sum_{k=0}^{\infty} \alpha_k(\boldsymbol{x}, t)\Psi_k(\xi_1,\ \xi_2, \ldots), \tag{3}$$

PDF: probability density function

PCE: polynomial chaos expansion

WH: Wiener-Hermite

GPC: generalized polynomial chaos

where the mode strengths are deterministic functions of space and time. Given the above chosen standard normal RVs ξ_i, the orthogonality of the Γ_p (or Ψ_k), with respect to the inner product $\langle u(\omega)v(\omega)\rangle = \int_\Omega u(\omega)v(\omega)dP$, requires that they be multivariate Hermite polynomials. Both the Γ_p and the corresponding Ψ_k may be generated from univariate Hermite polynomials using tensor products. Cameron & Martin (1947) proved the convergence of this Wiener-Hermite (WH) PCE for a general square-integrable stochastic process $X(\boldsymbol{x}, t, \omega)$.

In a practical computational context, one truncates the PCE in both order p and dimension n. The number of terms in the resulting finite PCE

$$X(\omega) \approx \sum_{k=0}^{P} \alpha_k \Psi_k(\xi_1, \ \xi_2, \ldots, \ \xi_n) \tag{4}$$

is $P + 1 = (n + p)!/n!p!$. The convergence rate of this representation depends on the shape of the function $X = f(\boldsymbol{\xi})$ (Boyd 1980). Exponential convergence is observed for RVs with the same density as that of $\boldsymbol{\xi}$. Xiu & Karniadakis (2002) developed generalized polynomial chaos (GPC) expansions by using a broader class of orthogonal polynomials in the Askey scheme (Askey & Wilson 1985, Schoutens 2000). Each family of orthogonal polynomials corresponds to a given choice of distribution for the ξ_i. Soize & Ghanem (2004) discuss chaos representations with an arbitrary probability measure (see also Wan & Karniadakis 2006b).

For a given $\boldsymbol{\xi}$ basis choice, the orthogonality of the polynomials $\Psi_k(\boldsymbol{\xi})$ with respect to the inner product on $L^2(\Omega)$ leads to

$$\begin{aligned}\langle \Psi_i \Psi_j \rangle &= \int \Psi_i\left(\boldsymbol{\xi}(\omega)\right) \Psi_j\left(\boldsymbol{\xi}(\omega)\right) dP(\omega) = \int \Psi_i(\boldsymbol{\xi})\Psi_j(\boldsymbol{\xi})\rho_\xi(\boldsymbol{\xi})\, d\boldsymbol{\xi} \\ &= \delta_{ij}\langle \Psi_i^2 \rangle,\end{aligned} \tag{5}$$

where $\rho_{\boldsymbol{\xi}}()$ is the probability density of $\boldsymbol{\xi}$. Orthogonality enables the evaluation of the truncated PC representation of an RV $u \in L^2(\Omega)$ by projecting onto the PC basis

$$\tilde{u}(\omega) = \sum_{k=0}^{P} u_k \Psi_k(\boldsymbol{\xi}), \quad u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{1}{\langle \Psi_k^2 \rangle} \int u(\boldsymbol{\xi}(\omega))\Psi_k(\boldsymbol{\xi}(\omega))\mathrm{d}P(\omega). \tag{6}$$

This orthogonal projection minimizes the mean-square error in $\tilde{u}$ on the space spanned by $\{\Psi_k\}_{k=0}^{P}$.

3.1. Evaluation of the Polynomial Chaos Expansion

One must evaluate PCEs for uncertain model parameters, whether RVs or random fields, from data before proceeding to the propagation of uncertainty through the model. Let us first consider the case of an RV $\lambda(\omega)$. If we presume that a parameter λ is independent of other model parameters and that it can be well represented using a PCE based on one dimension, ξ, then one can use the available measurements to construct its PDF and its cumulative distribution function (CDF), from which its PCE can be evaluated using transformations in probability space, as illustrated by Xiu & Karniadakis (2002). This technique relies on the inverse CDF and is feasible given the independence assumption. Conversely, if data are available on model parameters exhibiting underlying dependences, then, although one can construct multidimensional joint parametric CDFs from the data, they cannot be used following this inverse-CDF procedure to construct the corresponding PCEs, unless additional constraints are employed to resolve the indeterminacy of the inversion. Similar difficulties ensue if λ is represented in terms of a multidimensional PCE. Rather, one can find a PCE that provides an optimal representation of λ using regression or Bayesian (Jaynes 2003) model-fitting approaches.

We now consider the case of uncertain parameters represented as random fields $\kappa(\boldsymbol{x}, \omega)$, exhibiting spatial dependence. The case of a stochastic process, with time dependence, can be handled analogously. In this context, the spatial correlation structure of κ is evaluated from the available data to enable the construction of a PCE. The procedure uses the Karhunen-Loève (KL) expansion (Ghanem & Spanos 1991, Karhunen 1946, Loève 1948). We can represent any real-valued second-order random field $\kappa(\boldsymbol{x}, \omega)$ using the KL expansion as

KL: Karhunen-Loève

$$\kappa(\boldsymbol{x}, \omega) = \bar{\kappa}(\boldsymbol{x}) + \sum_{i=1}^{\infty} \eta_i(\omega)\sqrt{\lambda_i}\phi_i(\boldsymbol{x}), \tag{7}$$

where $\bar{\kappa}(\boldsymbol{x})$ is the mean of $\kappa(\boldsymbol{x}, \omega)$ at $\boldsymbol{x}$, and λ_i and $\phi_i(\boldsymbol{x})$ are the eigenvalues and eigenfunctions of the covariance kernel, respectively (Ghanem & Spanos 1991). The RVs $\eta_i(\omega)$ are uncorrelated with zero mean and unit variance and can be evaluated from the available data on κ. If κ is also a Gaussian process, then the η_i are Gaussian and independent. In practice, the KL expansion is truncated after a finite number of M modes,

$$\kappa(\boldsymbol{x}, \omega) \approx \bar{\kappa}(\boldsymbol{x}) + \sum_{i=1}^{M} \eta_i(\omega)\sqrt{\lambda_i}\phi_i(\boldsymbol{x}). \tag{8}$$

In the case of a Gaussian process, the KL expansion is readily a first-order WH PCE in M dimensions. In the general case of a non-Gaussian process, one can use the Rosenblatt (1952) transform to convert the η_i into a set of independent uniformly distributed RVs $\boldsymbol{\zeta}$. This enables the generation of $\boldsymbol{\eta}$ and $\boldsymbol{\zeta}$ samples in the same probability space and, via the inverse CDF, the construction of an expansion for κ in any PC basis (Das et al. 2008). When limited data prevent an accurate evaluation of the covariance, this overall procedure is infeasible, and one can resort again to regression or Bayesian methods (Daniels & Kass 1999, Ghanem & Doostan 2006).

4. POLYNOMIAL CHAOS UNCERTAINTY QUANTIFICATION METHODS

PC UQ methods have been developed both in the global context, employing spectral expansions spanning all of stochastic space, and in a local context, using localized spectral representations. In either case, one can propagate the PC-represented uncertainty through a model by using Galerkin projection to reformulate the governing equations into equations for the PC mode strengths, or by using numerical evaluation of the PC modes of the model outputs employing deterministic or random sampling of the original deterministic model/code. The latter approach has been termed nonintrusive, as the original code can be treated as a black box, whereas the former has been termed intrusive, as it requires new solvers/codes designed for the reformulated equation system. The advantage of the intrusive approach is that it directly finds the PC representation of model outputs by a one-time solution of the reformulated model. The advantage of the nonintrusive approach is that it uses the original model code, but this has to be balanced against the requisite computational cost of potentially many evaluations of the original model. These various methods are outlined below.

4.1. Global Methods

In the context of global PC representations, we first discuss nonintrusive PC UQ methods, followed by a discussion of intrusive methods.

4.1.1. Nonintrusive.

The nonintrusive propagation of uncertainty from model parameter λ to output u, where $u = \mathfrak{M}(\lambda)$, proceeds by the following collocation procedure, given an n-dimensional basis $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_n)$ and the known PCE for $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k(\boldsymbol{\xi})$:

MC: Monte Carlo

LHS: Latin hypercube sampling

1. One generates samples of $\boldsymbol{\xi}$, $\{\boldsymbol{\xi}^j\}_{j=1}^{N}$, according to the sampling strategy of interest.
2. For each sample $\boldsymbol{\xi}^j$, one evaluates $\lambda^j = \sum_{k=0}^{P} \lambda_k \Psi_k(\boldsymbol{\xi}^j)$ and $u^j = \mathfrak{M}(\lambda^j)$.
3. Using all N samples, one numerically evaluates the expectations for the Galerkin projection, $u_k = \langle u\Psi_k\rangle / \langle \Psi_k^2 \rangle$, $\forall k \in \{0, 1, \ldots, P\}$.
4. Given computed u_k values, one assembles the PCE $u = \sum_{k=0}^{P} u_k \Psi_k(\boldsymbol{\xi})$.

The computational cost of this strategy is typically dominated by the computation of $u^j = \mathfrak{M}(\lambda^j)$ for every λ^j. The most effective construction achieves a given accuracy in the estimated $\{u_k\}_{k=0}^{P}$ with the least number of samples. Sampling approaches may be classified generally as random or deterministic. Random sampling uses Monte Carlo (MC) evaluation of the projection integrals. Efficient MC sampling approaches make use of the structure of the integrand and/or the PDF of $\boldsymbol{\xi}$, $\rho_{\xi}(\boldsymbol{\xi})$. Specifically, Latin hypercube sampling (LHS) uses samples drawn from equiprobability partitioning of the support of $\rho_{\xi}(\boldsymbol{\xi})$. With $\boldsymbol{\xi}$ sampled randomly from its PDF, we have

$$u_k = \frac{\langle u\Psi_k\rangle}{\langle \Psi_k^2\rangle} = \frac{1}{\langle \Psi_k^2\rangle} \frac{1}{N} \sum_{j=1}^{N} u^j \Psi_k(\boldsymbol{\xi}^j), \qquad k = 0, 1, \ldots, P. \tag{9}$$

In general, however, the convergence rate of random sampling methods is slow, whether considering MC [$\varepsilon \approx \mathcal{O}(N^{-1/2})$], LHS, or other MC-based random sampling methods (Caflisch 1998), which renders them impractical for computationally intensive forward models. Conversely, they are well suited for high-dimensional problems. For example, the convergence rate of MC is independent of n, whereas LHS exhibits only weak dependence on it. Ghanem (1998a) demonstrated the use of MC collocation in conjunction with PC methods, and Ghiocel & Ghanem (2002) reported the use of LHS in this context.

As an alternative to random sampling (which does not take advantage of any smoothness in the integrand), deterministic sampling methods use quadrature for the numerical evaluation of projection integrals, presuming some polynomial order in the integrand. Using n-dimensional Gauss-Hermite quadrature, with q points in each dimension, we can compute the projection integrals for WH PC as

$$u_k = \frac{1}{\langle \Psi_k^2\rangle} \sum_{i_1=1}^{q} \cdots \sum_{i_n=1}^{q} u(x_{i_1}, \ldots, x_{i_n}) \Psi_k(x_{i_1}, \ldots, x_{i_n}) \prod_{k=1}^{n} w_{i_k}, \tag{10}$$

where $u(\boldsymbol{x}) = \mathfrak{M}(\lambda(\boldsymbol{x}))$, and $(x_k,\ w_k)$, $k = 1, \ldots, q$, are the one-dimensional (1D) Gauss-Hermite integration points and weights (Le Maître et al. 2002). These methods provide significant gains in efficiency over random sampling methods for low-dimensional systems. However, the exponential rise in the number of quadrature points with n [e.g., requiring $(p+1)^n$ points for p-th order chaos in Equation 10] renders such full tensor-product quadrature methods inefficient for high-dimensional problems. Alternatively, sparse-quadrature, Smolyak, or cubature methods (Smoljak 1963) combine a weak dependence on dimensionality with efficiencies gained from an assumed degree of smoothness (Nobile et al. 2008a,b).

Another class of nonintrusive collocation methods evaluates the PCE using a linear equation system, or regression, based on a select set of points, rather than by numerical evaluation of the Galerkin integrals. Tatang (1995) developed the deterministic equivalent modeling method along these lines using $(P+1)$ points, and Webster & Sokolov (2000) used this method in climate projections. A similar method was used by Isukapalli et al. (1998). More recently, Hosder et al. (2006) used this approach in the CFD context, employing $(P+1)$ collocation points to determine the $(P+1)$ PC mode strengths using a linear algebraic equation–system solution. Although this technique ensures an accurate representation at the collocation points, it has no explicit control on the error elsewhere. In contrast, MC and deterministic evaluation of the Galerkin projection integrals establish control on the mean-square error of the PC representation. Moreover, Hosder et al. (2006) point out the nonunique solution of the UQ problem using their approach, as choosing alternate collocation points can give a somewhat different solution. They later increased the number of collocation points to $2(P+1)$, for improved accuracy, resulting in a least-squares problem (Hosder et al. 2008).

ME-GPC: multielement generalized polynomial chaos

4.1.2. Intrusive. The intrusive approach relies on a Galerkin-projection reformulation of the original model equations to arrive at governing equations for the PC mode strengths of the model output (Ghanem & Spanos 1991). This can be easily illustrated for simple algebraic models $u = f(x; \lambda)$, where x is an uncertain input, and λ is an uncertain parameter. Let us consider, for example, $u = \lambda x$. Substituting the PCEs $x = \sum x_i \Psi_i$, $\lambda = \sum \lambda_i \Psi_i$, and $u = \sum u_j \Psi_j$; multiplying both sides by Ψ_k; taking expectations; and employing orthogonality; we get

$$u_k = \sum_{i=0}^{P} \sum_{j=0}^{P} \lambda_i x_j \frac{\langle \Psi_i \Psi_j \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, 1, \ldots, P. \tag{11}$$

The tensor

$$C_{ijk} = \frac{\langle \Psi_i \Psi_j \Psi_k \rangle}{\langle \Psi_k^2 \rangle} \tag{12}$$

is a known property of the basis, which can be computed once and stored, allowing the easy computation of the PCE of any two-term product. Three-term products, such as $u = \lambda x^2$, lead to $u_k = \sum_{i=0}^{P} \sum_{j=0}^{P} \sum_{r=0}^{P} \lambda_i x_j x_r \langle \Psi_i \Psi_j \Psi_r \Psi_k \rangle / \langle \Psi_k^2 \rangle$, which can be also similarly evaluated. To avoid the computational cost and complexity of dealing with high-dimensional tensors, a pseudospectral approach proceeds by the successive application of the two-term product formula, providing the PCE for $\tilde{u} = \lambda x$, followed by $u = \tilde{u} x$. Using the C_{ijk} tensor and the two-term product formula, one can deal with general polynomial functions $u = f(.;.)$, written generally as $u_k = \langle f \rangle_k = \langle f \Psi_k \rangle / \langle \Psi_k^2 \rangle$, $k = 0, 1, \ldots, P$. A wide class of other, nonpolynomial, functions can also be transformed in a similar manner (Debusschere et al. 2004). Ghanem & Spanos (1991) first outlined intrusive PC UQ constructions in the context of the stochastic Galerkin finite-element method (FEM).

4.2. Local Methods

The above PC representation uses global spectral expansions (e.g., for WH PC $\xi_i \in]-\infty, +\infty[$). This approach has limited utility when dealing with systems exhibiting bifurcations, with discontinuous $u = f(\boldsymbol{\xi})$, or with strong nonlinearities. This challenge has been suitably addressed by mapping and subdividing $\boldsymbol{\xi}$-space into a number of finite-sized domains, and employing local compact-support constructions on each.

Le Maître et al. (2004a,b, 2007) employed multiwavelet bases to arrive at local PC representations on block-decomposed stochastic domains. Practical use of these methods in multiple dimensions is best done with local representations based on rescaled Legendre polynomials with uniformly distributed $\boldsymbol{\xi}$ and first-level multiwavelet details. Le Maître et al. (2004b, 2007) used first-level details to guide the adaptive refinement of the block decomposition. The PC UQ problem in each block is decoupled from the rest and can be solved independently—intrusively or nonintrusively—until block refinement or coarsening is necessary. Wan & Karniadakis (2005) used adaptive block-decomposed multielement generalized polynomial chaos (ME-GPC) representations based on local Legendre-uniform GPC as well. Local representations have also been formulated using Galerkin finite-element discretizations of the global KL RV basis, without recourse to spectral PC representations (Deb et al. 2001). Babuška et al. (2004) further developed this methodology.

Stochastic representations employing local interpolating functions have also been used in the context of deterministic nonintrusive collocation. Mathelin & Hussaini (2003) evaluated PC algebra using stochastic collocation, employing local Lagrange interpolants (see also Mathelin et al. 2005). Xiu & Hesthaven (2005) used deterministic sampling over collocation points in random space with a Galerkin FEM. Babuška et al. (2007) used a collocation approach employing local interpolants over the span of the global KL RVs in a stochastic Galerkin FEM.

Matthies & Keese (2005), Xiu & Hesthaven (2005), and Ganapathysubramanian & Zabaras (2007) used sparse grids employed in cubature methods in the context of stochastic sparse-grid collocation, employing local interpolants. Nobile et al. (2008a,b) examined the use of sparse-grid collocation using isotropic/anisotropic Smolyak formulae.

5. POLYNOMIAL CHAOS UNCERTAINTY QUANTIFICATION IN COMPUTATIONAL FLUID DYNAMICS

PC UQ has found use in many CFD applications, including flow in porous media, incompressible and compressible flow, thermofluids, and reacting flow. The subsections below discuss examples of these applications, as well as unsteady dynamics.

5.1. Flow in Porous Media

Ghanem & Dham (1998) demonstrated the first use of KL/PC in uncertain porous media. Using FEM computations in this context, they described the transport of water and oil in an aquifer with uncertain spatial distribution of permeability. For illustration, let us consider the transient flow of water in a saturated medium. Using the continuity equation and Darcy's law (Bear 1972), we have

$$S\frac{\partial h(\boldsymbol{x},t)}{\partial t} - \nabla\cdot[K(\boldsymbol{x})\nabla h(\boldsymbol{x},t)] = g(\boldsymbol{x},t), \tag{13}$$

where S is the specific storage, $h(\boldsymbol{x},t)$ is the hydraulic head, $K(\boldsymbol{x})$ is the saturated hydraulic conductivity, and $g(\boldsymbol{x},t)$ is a fluid source/sink term, along with requisite initial and boundary conditions. Assuming known and deterministic S and $g(\boldsymbol{x},t)$, we let the conductivity be uncertain, represented by a random field with a KL expansion in terms of $\boldsymbol{\xi}=\{\xi_1,\xi_2,\ldots,\xi_n\}$, written in terms of PC as $K(\boldsymbol{x},\omega)=\sum_{i=0}^{P}K_i(\boldsymbol{x})\Psi_i(\boldsymbol{\xi}(\omega))$. Expressing the head as a PCE,

$$h(\boldsymbol{x},t,\omega)=\sum_{i=0}^{P}h_i(\boldsymbol{x},t)\Psi(\boldsymbol{\xi}(\omega)), \tag{14}$$

with unknown mode strengths $h_i(\boldsymbol{x},t)$, substituting into Equation 13, and dropping the $\boldsymbol{\xi}(\omega)$ for brevity, we get

$$S\sum_{i=0}^{P}\frac{\partial h_i(\boldsymbol{x},t)}{\partial t}\Psi_i - \sum_{i=0}^{P}\sum_{j=0}^{P}\Psi_i\Psi_j\nabla\cdot[K_j(\boldsymbol{x})\nabla h_i(\boldsymbol{x},t)] = g(\boldsymbol{x},t). \tag{15}$$

Given the orthogonality of the Ψ polynomials, we project on the k-th mode by multiplying with Ψ_k, taking the expectation, and dividing by $\langle\Psi_k^2\rangle$ to get

$$S\frac{\partial h_k(\boldsymbol{x},t)}{\partial t} - \sum_{i=0}^{P}\sum_{j=0}^{P}\nabla\cdot[K_j(\boldsymbol{x})\nabla h_i(\boldsymbol{x},t)]C_{ijk} = \frac{g(\boldsymbol{x},t)}{\langle\Psi_k^2\rangle}, \quad k=0,1,\ldots,P, \tag{16}$$

where $C_{ijk} = \langle \Psi_i \Psi_j \Psi_k \rangle / \langle \Psi_k^2 \rangle$ is a constant tensor, as introduced above. Thus, Equation 13 has been replaced by a larger system of coupled $(P+1)$ equations. This deterministic system for the $h_i(\boldsymbol{x}, t)$, with suitable initial and boundary conditions, has to be solved once to provide the PCE for $h(\boldsymbol{x}, t, \omega)$. We can generate realizations of $h(\boldsymbol{x}, t)$ with Equation 14 using sampled values of $\boldsymbol{\xi}$.

There has been much subsequent work on this problem. Ghanem (1998b) used this PC UQ construction in conjunction with MC for multiphase transport in random media. Lu & Zhang (2004) further studied this problem using MC, moment equations, and a combined KL–moment equation approach, with the KL–moment equation approach having significantly superior computational performance. Moreover, Tartakovsky & Xiu (2006) addressed the small-scale problem of Stokes flow in tubes with rough walls using uncertain geometry representations with transformations to deterministic rectangular domains.

5.2. Incompressible Flow

Le Maître et al. (2001) first investigated the use of PC UQ methods for incompressible laminar flow at moderate Reynolds numbers for 2D channel flow. Below, I present the basic derivation for the case with spatially uniform uncertain viscosity. With $\boldsymbol{u}$, p, and ν denoting velocity, pressure, and kinematic viscosity, respectively, this flow is governed by the incompressible Navier-Stokes equations

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \nu \nabla^2 \boldsymbol{u} \tag{17}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{18}$$

with deterministic initial/boundary conditions. We presume a known PCE for the kinematic viscosity, in terms of a single ξ, $\nu = \sum_{i=0}^{P} \nu_i \Psi_i(\xi)$. The associated PCEs for the velocity and pressure are $\boldsymbol{u}(\boldsymbol{x}, t) = \sum_{i=0}^{P} \boldsymbol{u}_i(\boldsymbol{x}, t)\Psi_i(\xi)$ and $p(\boldsymbol{x}, t) = \sum_{i=0}^{P} p_i(\boldsymbol{x}, t)\Psi_i(\xi)$, where $\boldsymbol{u}_i$ and p_i are the unknown PC mode strengths. Introducing these expansions into the governing equations results in

$$\sum_{i=0}^{P} \Psi_i \frac{\partial \boldsymbol{u}_i}{\partial t} + \sum_{i=0}^{P} \sum_{j=0}^{P} \Psi_i \Psi_j (\boldsymbol{u}_i \cdot \nabla)\boldsymbol{u}_j = -\sum_{i=0}^{P} \Psi_i \nabla p_i + \sum_{i=0}^{P} \sum_{j=0}^{P} \Psi_i \Psi_j \nu_i \nabla^2 \boldsymbol{u}_j, \tag{19}$$

$$\sum_{i=0}^{P} \Psi_i \nabla \cdot \boldsymbol{u}_i = 0. \tag{20}$$

Multiplying Equation 19 by Ψ_k, making use of orthogonality, and dividing by $\langle \Psi_k^2 \rangle$, for $k = 0, \ldots, P$, we get

$$\frac{\partial \boldsymbol{u}_k}{\partial t} + \sum_{i=0}^{P} \sum_{j=0}^{P} (\boldsymbol{u}_i \cdot \nabla)\boldsymbol{u}_j C_{ijk} = -\nabla p_k + \sum_{i=0}^{P} \sum_{j=0}^{P} \nu_i \nabla^2 \boldsymbol{u}_j C_{ijk}. \tag{21}$$

A similar treatment for the velocity divergence constraint gives

$$\nabla \cdot \boldsymbol{u}_k = 0, \quad k = 0, \ldots, P. \tag{22}$$

The original system of three momentum equations and the continuity constraint has been transformed into a larger system of $3(P+1)$ coupled equations in terms of the PC mode strengths of the velocity and pressure fields, along with $(P+1)$ constraints on the velocity mode strengths. Le Maître et al. (2001) showed how this system can be solved using projection methods, involving a decoupled set of $(P+1)$ elliptic problems for the pressure field.

Figure 1 shows sample results for 2D rectangular channel flow with uncertain viscosity, following Le Maître et al. (2001). This study used a uniform inflow velocity, with nonslip sidewalls

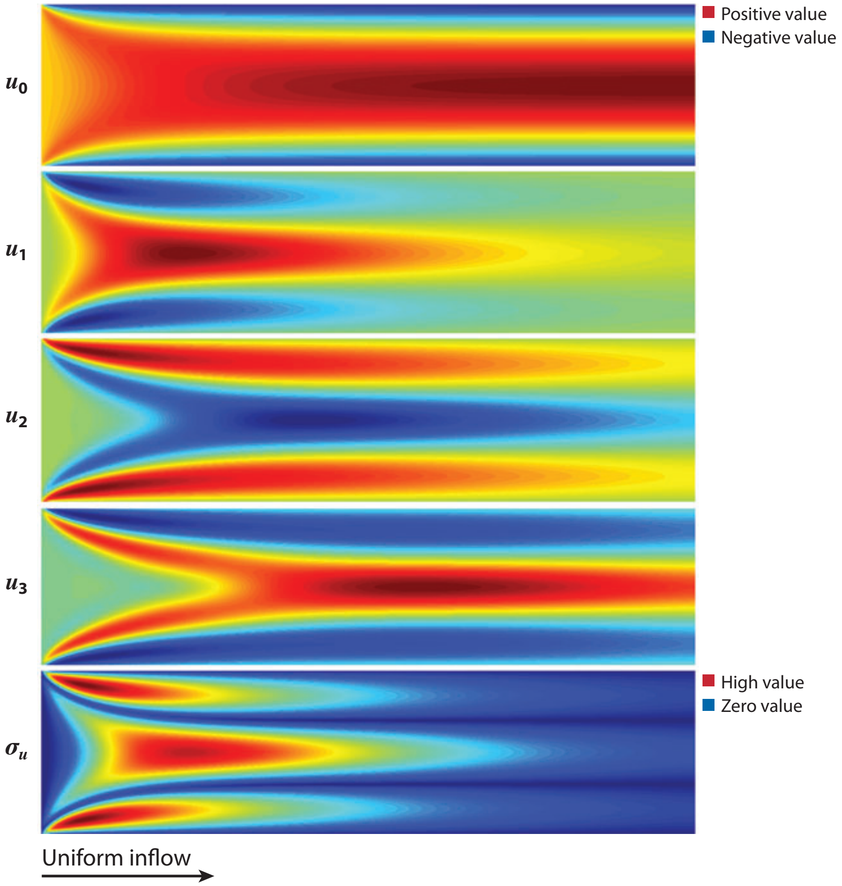

Figure 1

Two-dimensional channel flow with uncertain viscosity. The plot shows the polynomial chaos mode strengths of the horizontal u velocity field, from top to bottom: u_0, u_1, u_2, and u_3, as well as the standard deviation σ_u of the u velocity (*bottom frame*). Uniform inflow is at the left edge. Positive values of $\{u_1, u_2, u_3\}$ are shown in red, whereas negative values are shown in blue. For σ_u, high values appear in red, and zero σ_u is in blue.

and an uncertain Gaussian viscosity, and a third-order 1D PCE. The flow has a Reynolds number $Re = 81$ and is steady and laminar. The mean field (u_0) reveals the expected growth in the velocity along the channel centerline with downstream distance, as the flow transitions from the uniform inlet velocity profile to a parabolic profile further downstream. The field plots for the individual modes and standard deviation $\sigma_u = (\sum_{k=1}^{P} u_k^2 \langle \Psi_k^2 \rangle)^{\frac{1}{2}}$ exhibit significant structure. The inflow edge has, by definition, a deterministic velocity, hence zero σ_u. As one proceeds into the channel, the consequences of uncertain viscosity appear as a central region of large σ_u, as well as two lobes in the developing boundary layers along either wall.

Xiu & Karniadakis (2003) used GPC for UQ in modeling incompressible channel flow and for flow around a circular cylinder. Narayanan & Zabaras (2005) employed global GPC UQ in the context of stabilized FEM solutions of incompressible channel and driven cavity flows. Le Maître (2006) used intrusive PC for inviscid incompressible flow around an airfoil, with a Lagrangian vortex model, and Le Maître & Knio (2007) introduced a stochastic particle-mesh vortex method for incompressible flow computations with PC UQ.

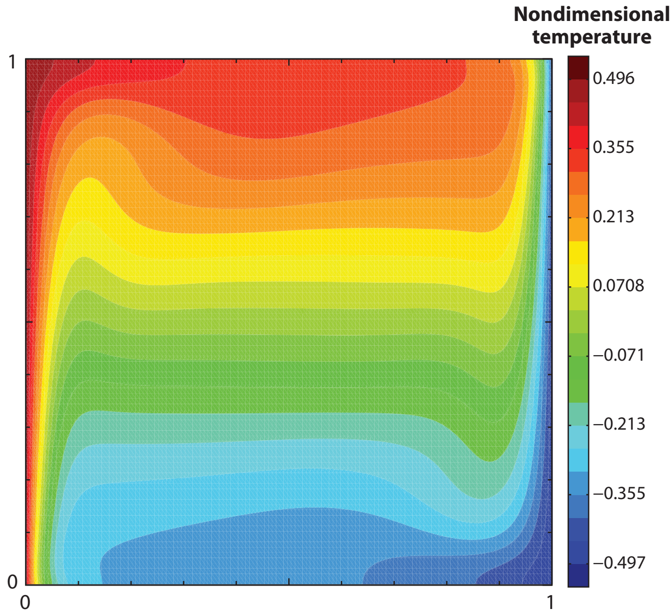

Figure 2

Mean temperature field in a differentially heated cavity. The scale on the right indicates the range of low- to high-nondimensional temperature. The right wall temperature is cold, with prescribed uncertainty, whereas the left wall is hot and deterministic. The top and bottom walls are adiabatic. Figure reproduced with permission from the *Journal of Computational Physics*.

5.3. Thermofluid Flow

Le Maître et al. (2001) studied uncertain thermofluid flows using intrusive WH PC, in the context of incompressible channel flow with temperature-dependent viscosity. They later applied this construction in modeling natural convection in a differentially heated cavity with adiabatic top and bottom walls and cold/hot sidewalls in the Boussinesq limit (Le Maître et al. 2002). Nominal conditions corresponded to a steady laminar recirculating flow regime. They presumed an uncertain cold wall temperature and modeled it as a random process with a specified correlation length, which they represented using a KL approach. The mean temperature field exhibits two layers parallel to the vertical walls and horizontal stratification in the vertical direction (**Figure 2**). The temperature standard-deviation field has a similar topology, with a maximum on the (right) cold wall, at which the uncertain temperature is imposed, and a zero minimum at the (left) hot wall, at which a deterministic high temperature is imposed. **Figure 3** shows the mean horizontal and vertical velocity profiles at a number of stations in the cavity, with superimposed 6σ uncertainty error bars. The mean velocity field highlights the bulk average circulation of the flow in the clockwise direction. Uncertainty grows in both the temperature and the velocity fields as fluid moves downward along the right wall. This growth is driven by the uncertainty in the temperature on that wall, and uncertainty is convected along with the circulating mean velocity field. Le Maître et al. (2004c) extended this study to the non-Boussinesq limit, implementing the full variable-density low-Mach-number equations, again using intrusive KL-PC. Numerical stability required discrete global mass conservation in the stochastic equations to ensure the solvability of the elliptic equations for the pressure modes.

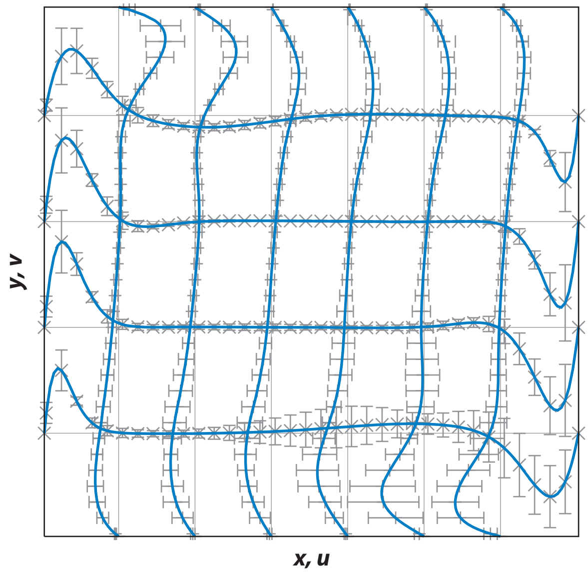

Figure 3

Horizontal and vertical velocity profiles at select stations in the differentially heated cavity, with superposed 6σ uncertainty error bars. Figure reproduced with permission from the *Journal of Computational Physics*.

Le Maître et al. (2004a) also studied Rayleigh-Bénard flow in the Boussinesq limit using PC UQ. In this context, they considered a cavity with a heated bottom wall. Above a critical Rayleigh number, the system transitions from a conductive to a convective heat-transfer mode, as the instability of the flow leads to convective motion. Uncertainty is prescribed in the bottom wall temperature. This study explored the performance of a global Wiener-Legendre GPC construction versus a local Wiener-Haar scheme employing a Haar wavelet basis. The results demonstrated the superior performance of the local construction when the parametric uncertainty spans the bifurcation corresponding to the critical Rayleigh number. The failure of the global spectral expansion to represent a bifurcation in stochastic space is not surprising. The local construction dealt with the bifurcation effectively. Asokan & Zabaras (2005) reached similar conclusions in this system using GPC UQ in a stabilized, variational multiscale FEM.

Wan & Karniadakis (2006b) used ME-GPC for UQ in incompressible flow and heat transfer in a 2D channel over an open cavity with a spectral element solver. At high Reynolds number, large stochastic perturbations were evident, and the local ME-GPC construction was more efficient than the global GPC.

5.4. Reacting Flow

Reacting flow presents serious challenges to PC UQ, through the high dimensionality associated with many uncertain parameters and the strong nonlinearity of chemical reactions. Phenix et al. (1998) first used PC UQ in isothermal chemical ignition in their deterministic equivalent modeling–method approach, focusing on supercritical water oxidation. With this chemical model, Reagan et al. (2003) employed nonintrusive WH PC with LHS in ignition and 1D flames in isothermal supercritical water oxidation. They also later computed uncertain sensitivity coefficients from the PC results (Reagan et al. 2005).

Reagan et al. (2004) presented an intrusive reformulation of a general chemical kinetic source term using pseudospectral PC, highlighting the need for high PC order to ensure the positivity of species concentrations and to maintain stability under fast rates of amplification of uncertainty. Increasing order by itself was not sufficient, however, as the required order became exorbitantly high. These challenges were addressed using local multiwavelet PC by Le Maître et al. (2007).

Debusschere et al. (2003) also studied UQ in electrochemical reacting flows in microchannels with electroosmotic pumping using WH PC. This construction coupled the Navier-Stokes equations with species-conservation equations, including the electrokinetic body force, and electrostatics. The chemical model involved both electrolytic buffer reactions and protein-labeling chemistry.

5.5. Compressible Flow

Compressible flow presents unique challenges for PC UQ, particularly with regard to shock discontinuities. This challenge was amply discussed by Chen et al. (2005), who used an intrusive GPC UQ in a 1D nonlinear inviscid Burgers equation model of steady-state isentropic nozzle flow, with uncertain initial conditions leading to uncertainty in shock location. They showed that, although the velocity field exhibits a discontinuity in the spatial dimension x at the shock location, the dependence of the velocity PCE mode strengths on x is smooth. It is the discontinuity of the solution in stochastic space, for a given x, that leads to convergence difficulties with global PC. In this context, Chen et al. (2005) indicate that filtering is necessary for numerical stability. When the uncertainty in the initial condition was low, they observed high accuracy in the predicted uncertain shock location. Otherwise, their results exhibit slow convergence of the global PCE, requiring many terms, without attaining high accuracy.

Perez & Walters (2005) studied other canonical compressible flow problems, such as the supersonic flow over a wedge (which exhibits an oblique shock) and that over an expansion corner (which exhibits a Prandtl-Meyer expansion wave), using intrusive PC UQ. Lin et al. (2006) also studied the supersonic wedge flow using intrusive GPC and ME-GPC constructions. In the context of both the supersonic wedge and expansion-corner problems, Hosder et al. (2006) evaluated the efficacy of nonintrusive collocation (similar to the deterministic equivalent modeling method) PC UQ constructions compared to MC computations. Computations revealed strongly non-Gaussian statistics in locations near the shock in the wedge flow, which required high PC order to reduce the error in the collocation results. The expansion-corner flow, conversely, exhibited largely Gaussian statistics, and relatively small collocation error, everywhere. Hosder et al. (2008) used an extension of this scheme for UQ in flow around a transonic wing.

Mathelin et al. (2004) used intrusive WH PC for UQ in a turbulent, compressible supersonic quasi-1D nozzle flow. Challenges with extending the intrusive construction to nonpolynomial nonlinearities and discontinuous functions (and poor performance under strong nonlinearity) drove Mathelin & Hussaini's (2003) development of a local stochastic, collocation, nonintrusive PC UQ scheme. They demonstrated this construction in the context of a stochastic Riemann problem, involving a discontinuous field variable leading to the generation of a shock wave, rarefaction, and expansion fan. Mathelin et al. (2003) used this scheme for UQ in the quasi-1D nozzle flow, comparing it to MC methods and intrusive PC and demonstrating its accuracy and computational efficiency in this problem (see also Mathelin et al. 2005).

5.6. Unsteady Dynamics

Flow unsteadiness presents a significant challenge for PC UQ. Wiener (1939) had considered PCEs as potential means to study turbulent flow. However, any finite PCE fails to represent turbulence. Orszag & Bissonnette (1967) found that nonlinearities propagate energy into higher-order terms. Crow & Canavan (1970) and Chorin (1974) highlighted the failure of finite WH expansions to represent the turbulent energy cascade. More recently, Hou et al. (2006) returned to this topic, employing an adaptive strategy for the retention of significant high-order PC terms, due to Li & Ghanem (1998), finding that long-term dynamics remain a challenge.

Oscillatory vortex shedding behind a circular cylinder was studied by Xiu et al. (2002) using PC UQ and by Lucor & Karniadakis (2004) and Narayanan & Zabaras (2005) using GPC. Wan & Karniadakis (2006a), employing a 1D advection equation model, showed that the time horizon for given accuracy and PC order is extended by a factor of N when a uniform mesh of N stochastic elements is used in ME-GPC versus global GPC. They demonstrated accurate time-horizon extension with ME-GPC in the flow around a cylinder but cautioned regarding the cost of increased dimensionality in time.

Oscillatory dynamics have also been studied with a focus on airfoil limit-cycle oscillations. Pettit & Beran (2004) explored the utility of global PC for representing uncertain limit-cycle oscillations. They observed large errors for long time horizons, resulting from finite PC order. A sinusoid-model study, with uncertain frequency, outlined the increased nonlinearity/frequency of the ξ dependence of the requisite PCE in time, thus requiring higher order. Pettit & Beran (2006) used local Wiener-Haar PC (Le Maître et al. 2004a) for limit-cycle-oscillation analysis, which dealt well with the Hopf bifurcation and its associated discontinuity in ξ. Although high wavelet resolution improved accuracy for a given time horizon, nonlinear oscillators still showed deterioration of time accuracy for long times.

6. CONCLUSION

This review discusses the basic principles and utilization of PC UQ methods in CFD. These methods provide significant performance and utility in a range of CFD applications. At the same time, there are remaining challenges, mostly associated with high dimensionality and with long time horizons in unsteady flow. These topics are the subject of ongoing research.

DISCLOSURE STATEMENT

The author is not aware of any biases that might be perceived as affecting the objectivity of this review.

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