Proceedings of the XII International Symposium on Dynamic Problems of Mechanics (DINAME 2007),
P.S.Varoto and M.A.Trindade (editors), ABCM, Ilhabela, SP, Brazil, February 26 - March 2, 2007

Predictive Science: A Confluence of Verification, Validation and Uncertainty Quantification

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Abstract: The validation of predictive models entails determining whether a certain model is suitable to a certain task. The suitability criterion is construed as quantifying the closeness of the model-based predictions to either existing or potential experimental evidence.
A constructive approach is presented to the task of validating predictive models. A mathematical framework is delineated that permits the formulation of meaningful questions in connection with the validation prcess. These questions may relate to the validity of a certain model, or to whether a non-validated model can be validated, and if so then at what expense. In this latter case, computable actions to ensure validation are developed.
The mathematical framework permits the formulation of the problem as that of approximation over a product measure space. This approach permits the extension of concepts from adaptive error estimation as developed for PDE's to the realm of model validation. Improving the accuracy of predictions, through mesh refinement, adaptive time-stepping, or adaptive sampling, for example, is now supplemented by a refinement of the data upon which the model is based.
This framework permits the blending of experimental data with model-based data. This has significant consequence for implementation of performance-based design concepts, the analytical certification of components and systems, as well as for optimizing the allocation of resources between experimental and computational efforts.
Challenges in the design and accreditation of dynamical systems in the presence of significant uncertainty are discussed. It is demonstrated how several components of uncertainty that are ubiquitous in these problems can be simultaneously treated using a rigorous and consistent mathematical description.

Keywords: Uncertainty quantification, Polynomial Chaos, Model validation, Stochastic analysis

INTRODUCTION

The single most significant driver behind high performance computing is the vision of a computational laboratory that is a reliable surrogate to a physical laboratory. Gains associated with fulfilling this vision are significant to all aspects of societal well-being. While Moore's law has served to produce computers that are necessary to achieve this vision, the gap remains wide; there is a growing consensus in the science community that algorithmic and conceptual developments are essential for narrowing it. A significant obstacle in fulfilling this vision is the presence of uncertainties at every juncture in the computational process, from the physical reality that is being approximated, all the way to round-off errors on the computational hardware. The need to address the challenges represented by this obstacle has grown more pressing in light of the increased reliance on very high performance computational resources and the associated expectation of accuracy in predictions.

Uncertainty is ubiquitous in the natural, engineered, and social environments. Devising rationales for explaining it, strategies for its integration into scientific determinism and mitigating its consequences has been an active arena of rational endeavor where many scientific concepts have taken turn at fame and infamy. Far from being a static concept, uncertainty is the complement of knowledge, and as thus, continually adapts itself to knowledge, feeding on its evolution to redefine its claim over science.

Mechanics is a framework for applying deductive and mathematical reasoning to enhance our understanding of the physical world. Thus, far from being accidental, the interaction of mechanics and uncertainty is rather by design, as they both mold the physical world in a complementary fashion. The substance of this interaction is attested to by the simultaneous evolution of mechanics and rational models of uncertainty as embodied, for example, in the contributions of Gauss, Euler, Legendre, Laplace, Einstein, Feynman, and vonMises.

Two driving forces behind a significant portion of current scientific research can be associated with technological developments in the areas of computing and sensing. Indeed, it has only recently become possible to resolve, numerically, very complex models of physical phenomena, as well as to probe these phenomena over length-scales that span orders of magnitude. This facility for doing science significantly changes the realm over which uncertainty can claim a hold, and merits a reconsideration of the scientific questions enabled through uncertainty modeling.

The concept of Model Validation has proven quite useful in the present context. Model validation is the process for

establishing sufficient confidence in a computational prediction to allow a decision to be made using that prediction. The ultimate goal of validation is to achieve quantitatively accurate predictions for complex physical scenarios via modeling and computational simulation for which no other mathematical descriptions, such as closed-form solutions, exist.

Connections to these physical scenarios can only be achieved through experiments and any observations made during their execution. Furthermore, limitations on the scale, scope, and relevance of observations of physical phenomena inject elements of uncertainty into any modeling endeavor. Thus, sophisticated UQ-enabled syntheses of observations into the associated models are required.

This "Model Validation" driver dictates the need for mathematically modeling physical observations in a manner that is as consistent as possible with numerically simulated reality. It also dictates the need to quantify the proximity of model-based predictions to physical reality, taking into account, in a computable manner, the main sources of discrepancy. Thus, having selected a set of physics to describe the problem, a well-posed question is formulated regarding the extent to which predictions using these physics can be close to reality. The answer to this question presents the limit on predictability using that particular model.

PROBABILISTIC CONTEXT

This paper focuses on a particular class of recent developments related to the quantification, propagation, and management of uncertainty, using a probabilistic framework. An attempt is made at presenting a formalism that facilitates the adaptive quantification of uncertainty and of its effect on mechanics-based predictions. In addition to the more traditional quest for estimating the probability of extreme events such as failure, attention is given to estimating the confidence in model predictions and to adaptive schemes for improving this confidence through model refinement (mechanistic and numerical) as well as data refinement. The possibility of performing such an adaptation can play a significant role in shaping performance-based design practice in science and engineering by quantifying the information, and its associated worth, required to achieve a target confidence in the predicted behavior of some contemplated design. The concept of combined stochastic-deterministic error and its estimation is introduced that permits the development of optimal numerical optimization strategies such as adaptive mesh refinement that are consistent with the level of accuracy justified by available data. Concepts are presented that guide the simultaneous refinement of mesh and data. The uncertainty quantification, propagation and management framework to be presented is based on Hilbert space representations and projections of random functions. This permits the framework to be integrated with other Hilbert space representations used in computational mechanics and signal analysis.

A mapping, $\mathscr{M}$, can be conceptually defined between events corresponding to random parameters and events corresponding to measurable outputs. This mapping takes measurable subsets $\mathscr{T}$ into measurable subsets $\mathscr{Q} = \mathscr{M}(\mathscr{T})$. A measure can be associated to each subset $\mathscr{T}$ reflecting a subjective assessment of the likelihood of that event occurring. The corresponding measure on $\mathscr{Q}$ is uniquely computable by the mapping $\mathscr{M}(.)$. In order to facilitate the analysis, and given that most measurable events of interest refer to numerical measurements, it is usually convenient to work on measures defined on the real line. Random variables provide a mechanism for effecting that, since they are defined as mappings from the set of basic events onto the real line. Loosely speaking, each of the events $\mathscr{T}$ and $\mathscr{Q}$ are mapped, through appropriate random variables, into subsets of the real line, the measure of which are identified with the measure of the corresponding event. The mapping $\mathscr{M}(.)$ can now be replaced by a new mapping $\mathscr{N}(.)$ between the random variables. It is usually this mapping that is dealt with in the context of mechanistic modeling. It can be shown that, as mappings go, second order random variables have a number of very interesting properties, so much so that they collectively form a Hilbert space when endowed with the inner product defined through the operation of statistical correlation. This Hilbert space structure is very convenient as it forms much of the foundation of deterministic numerical analysis: projections on subspaces as well as convergent approximations can now be meaningfully defined and implemented.

Contributions to formulating and solving the problem can be made at a number of key steps. Firstly, events $\mathscr{Q}$ of interest to a given problem must be identified. These consist, for example, of failure events, of levels of exceedance, or of some death/birth events. A mathematical description of the set to which these events belong must be adopted that is rich enough to distinguish between the various events of interest. Moreover, a corresponding, consistent, topology over the set to which events $\mathscr{T}$ belong must be identified that is commensurate with available instrumentation technology. Secondly, the measure on the various events $\mathscr{T}$ must be estimated. In a probabilistic framework such as the present one, this amounts to estimating the probability measure of the various events. The outcome of this task, and hence the confidence in the overall uncertainty quantification and propagation process, depends in no small measure on the choice of model and data used to calibrate the associated parameters. The ability to adaptively update the probabilistic characterization of the associated random variables are shown to be a significant feature of the framework presented in the paper. Thirdly, an algorithm for propagating the uncertainty in the parameters into uncertainty in the predictions must be developed. This algorithm should clearly take into consideration the mechanistic model adopted for the problem, the accuracy with which numerical predictions of this model can be resolved, as well as the practical questions that the uncertainty analysis is trying to address. Obviously, this uncertainty propagation task can be performed, at least conceptually, by relying on the Monte Carlo simulation (MCS) paradigm. It is shown that methods can be developed that generalize MCS, increasing its

efficiency while providing it with improved error estimation capabilities, that are as much based on the mechanics of the problem as on statistics of the data. Based on the above, a solution of the following form is sought,

$$u = \hat{u} + \varepsilon_h + \varepsilon_p + \varepsilon_d$$

where $\hat{u}$ is some computed prediction of the solution, ε_h, ε_p, and ε_d are error estimators that can be controlled by refining the numerical approximations, refining the probabilistic approach, and refining the data, respectively. Adaptive techniques for controlling ε_h are well established in deterministic computational mechanics. The formalism presented in this paper demonstrates the development of similar adaptation schemes for ε_p and ε_d. It is clear that the certification of the predicted solution $\hat{u}$ to be within a specified tolerance requires the rational control of all three error terms. Selection between competing models can then be made by identifying that model which achieves its target error reduction within specified limits on computational and data collection resources. The problem can then be described as follows: The model parameters, as estimated from data and modeled as random variables or processes, live in the Hilbert space $\mathscr{H}_{\mathscr{G}}$. Assuming the data to be well defined in a probabilistic sense provides a full characterization of this space, in which a set of basis functions, ξ_i , will have to be identified. This will be accomplished using the Karhunen-Loeve expansion. The state of the system, again modeled as a random variable or process, resides in the Hilbert space $\mathscr{H}_{\mathscr{L}}$. A set of basis functions, ψ_i, will also be identified in this space, which in general will be different from the basis ξ_i since this latter one spans only a subset of the space of second order random variables, namely those that characterize the data. Identifying a basis for the space $\mathscr{H}_{\mathscr{L}}$ will be accomplished using the Chaos theory of Wiener. The solution of the problem can then be characterized by its projection on this basis. A Galerkin scheme is used to formulate this projection on a finite dimensional subspace, and equations governing the evolution of the associated coefficients are obtained. This form of characterizing the solution of a probabilistic problem, permits the propagation of the uncertainty with minimal loss of information. Indeed, the solution is being represented as a stochastic process, and not as an integrated norm of that process. Moreover, the representation used for that process, namely the basis set ψ_i is appropriate for representing both the input and output of a mechanistic model, thus eliminating the need for significant post-processing and the associated loss of information.

Solving stochastic PDE's using the polynomial chaos formalism consists of two parts. The first part involves representing the stochastic processes involved. These include the processes for the model parameters as well as the processes for the unknown field quantities. The second part involves formulating the numerical problem for estimating the representation of the unknown field quantities. This review is therefore structured in two parts, describing these two components.

ORTHOGONAL REPRESENTATIONS OF STOCHASTIC PROCESSES

Two representations in particular are described next. These are the Karhunen-Loeve and the Polynomial Chaos expansions. The first one is a modal-based representation of stochastic process along eigenvectors of its covariance kernel, while the second one is a polynomial representation of random functions with respect to multidimensional polynomials in gaussian variables.

Karhunen-Loeve Expansion

The Karhunen-Loeve (KL) expansion provides a mean-square optimal representation of a stochastic process in terms of a denumerable set of random variables. While the joint measure on these random variables is usually cumbersome to manipulate, these variables are used to delineate an optimal approximation subspace. This section provides technical background on the KL expansion.

Let $\{\boldsymbol{Z}(\boldsymbol{\zeta}), \boldsymbol{\zeta} \in B\}$ be a second-order centered stochastic process, defined on probability space $(\mathscr{A}, \mathscr{T}, P)$, and indexed by a bounded set B of $\mathbb{R}^d$ with values in $\mathbb{R}^m$. The matrix-valued correlation function of $\boldsymbol{Z}$ is thus given by,

$$\boldsymbol{R}_{\boldsymbol{Z}}(\boldsymbol{\zeta}, \boldsymbol{\zeta}') = E\left\{\boldsymbol{Z}(\boldsymbol{\zeta})\boldsymbol{Z}(\boldsymbol{\zeta}')^T\right\} , \tag{1}$$

and is assumed to be such that

$$\int_B \int_B \|\boldsymbol{R}_{\boldsymbol{Z}}(\boldsymbol{\zeta}, \boldsymbol{\zeta}')\|_{HS}^2 \, d\boldsymbol{\zeta}' \, d\boldsymbol{\zeta} < \infty , \tag{2}$$

where $\|.\|_{HS}$ is the Hilbert-Schmidt norm. For instance, since B is a bounded set of $\mathbb{R}^d$, condition defined by equation (2) is satisfied if $\boldsymbol{Z}$ is a mean-square continuous stochastic process on B. Here $E\{\}$ denotes the operator of mathematical expectation. Let then $\mathbb{V} = L^2_{d\boldsymbol{\zeta}}(B, \mathbb{R}^m)$ be the Hilbert space of $\mathbb{R}^m$-valued square-integrable functions on B equipped with the inner product

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\mathbb{V}} = \int_B \langle \boldsymbol{u}(\boldsymbol{\zeta}), \boldsymbol{v}(\boldsymbol{\zeta}) \rangle_{\mathbb{R}^m} \, d\boldsymbol{\zeta} . \tag{3}$$

Due to equation (2), the linear operator $\boldsymbol{R}_{\boldsymbol{Z}}$ defined by the following bilinear form on $\mathbb{V} \times \mathbb{V}$,

$$\langle \boldsymbol{R}_{\boldsymbol{Z}}\boldsymbol{u},\boldsymbol{v}\rangle_{\mathbb{V}} = \int_B \int_B \langle \boldsymbol{R}_{\boldsymbol{Z}}(\boldsymbol{\zeta},\boldsymbol{\zeta}')\boldsymbol{u}(\boldsymbol{\zeta}'),\boldsymbol{v}(\boldsymbol{\zeta})\rangle_{\mathbb{R}^m}\, d\boldsymbol{\zeta}'\, d\boldsymbol{\zeta} \tag{4}$$

is a Hilbert-Schmidt operator. Consequently, the eigenvalue problem,

$$\boldsymbol{R}_{\boldsymbol{Z}}\boldsymbol{\phi} = \lambda\ \boldsymbol{\phi} \tag{5}$$

has a sequence of real positive eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \to 0$ such that $\sum_{j=1}^{\infty} \lambda_j^2 < \infty$. The associated eigenfunctions form a Hilbertian basis of $\mathbb{V}$. In this case, the Karhunen-Loeve decomposition of stochastic process $(\boldsymbol{Z}(\boldsymbol{\zeta}), \boldsymbol{\zeta} \in B)$ can be written as

$$\boldsymbol{Z}(\boldsymbol{\zeta}) = \sum_{j=1}^{\infty} \sqrt{\lambda}_j\ \eta_j\ \boldsymbol{\phi}_j(\boldsymbol{\zeta}) \tag{6}$$

with

$$\eta_j = \frac{1}{\sqrt{\lambda_j}} \langle \boldsymbol{Z},\boldsymbol{\phi}\rangle_{\mathbb{V}}\ , \tag{7}$$

where the sequence of random variables $\{\eta_j\}$ is such that,

$$E\{\eta_j\} = 0 \qquad E\{\eta_i\eta_j\} = \delta_{ij}\ . \tag{8}$$

Truncating the KL expansion at the μ^{th} term defines the approximation $\boldsymbol{Z}^{\mu}(\boldsymbol{\zeta})$ as,

$$\boldsymbol{Z}^{\mu}(\zeta) = \sum_{j=1}^{\mu} \sqrt{\lambda}_j\ \eta_j\ \boldsymbol{\phi}_j(\boldsymbol{\zeta})\ . \tag{9}$$

For details on the K-L expansion applied to the stochastic finite element method (SFEM), including solving the integral eigenvalue problem over complex geometries, we refer to (Ghanem and Spanos, 1991).

For the very important case where the uncertainty appears as a random variable, and not as a random process, the Karhunen-Loeve expansion reduces to a single term. The present formulation, clearly, permits the treatment of this very important and practical situation as a special case of the more general procedure. It should be noted that in the case of stochastic processes, it is important that the Karhunen-Loeve expansion produces a probabilistic characterization of processes that are physically admissible. Two classes of approaches have been pursued to that end by various researchers. The first class sets mathematical conditions on the components in the expansion so as to ensure the almost sure ellipticity of the associated operators (Babuska and Chantzipantelidis, 2002). The second class of approaches to this problem synthesizes a Karhunen-Loeve decomposition from observed data (Shi 2003; Shi and Ghanem, 20007). A Karhunen-Loeve expansion with a few terms is thus obtained, where each term represents the "measured" contribution to uncertainty from a given scale. The KL expansion is thus viewed as an analytical procedure for packaging information observed at different scales, including the scale-dependent scatter in that information. Given the physical-based connotation of this construction procedure, it can be expected that the resulting stochastic process will adhere to all the necessary physical constraints, including ellipticity of the governing operator when this property is applicable.

Polynomial Chaos Expansion

Consider a physical system featuring random uncertainties in some of the parameters of its mathematical model. The random uncertainties are identified with the p basic vector-valued random variables $\boldsymbol{Z}^1,\ldots,\boldsymbol{Z}^p$. The solution describing the behavior of the physical system is a $\mathbb{R}^N$-valued random variable $\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{Z}^1,\ldots,\boldsymbol{Z}^p)$ in which $\boldsymbol{f}$ is a nonlinear mapping. It will be assumed, without loss of generality that vector-valued random variables $\boldsymbol{Z}^i$ are uncorrelated (which can be easily achieved through a Gram-Schmidt procedure) and that they are statistically independent for different i (this implies that different parameters in the model are independent), so that

$$P_{\boldsymbol{Z}^1,\ldots,\boldsymbol{Z}^p} = P_{\boldsymbol{Z}^1} \otimes \ldots \otimes P_{\boldsymbol{Z}^p}\ , \tag{10}$$

where $P_{\boldsymbol{Z}^j}$ is the probability distribution of random variable $\boldsymbol{Z}^j$. Note that the chaos representation of random variable $\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{Z}^1,\ldots,\boldsymbol{Z}^p)$ is obtained by representing $(\boldsymbol{x}^1,\ldots,\boldsymbol{x}^p) \mapsto \boldsymbol{f}(\boldsymbol{x}^1,\ldots,\boldsymbol{x}^p)$ on a Hilbertian basis. Since $\boldsymbol{Z} = (\boldsymbol{Z}^1,\ldots,\boldsymbol{Z}^p)$ is a random variable with values in a finite-dimensional vector space, the associated chaos representation of $\boldsymbol{Y}$ is said to be finite-dimensional. The chaos representation of random variable $\boldsymbol{Y} = \boldsymbol{f}(\boldsymbol{Z}^1,\ldots,\boldsymbol{Z}^p)$ is then given as (Soize and Ghanem, 2004),

$$\boldsymbol{Y} = \sum_{\boldsymbol{\alpha}^1 \in \mathbb{N}^{m_1}} \cdots \sum_{\boldsymbol{\alpha}^p \in \mathbb{N}^{m_p}} \boldsymbol{f}_{\boldsymbol{\alpha}^1 \ldots \boldsymbol{\alpha}^p} \, \phi^1_{\boldsymbol{\alpha}^1}(\boldsymbol{Z}^1) \times \ldots \times \phi^p_{\boldsymbol{\alpha}^p}(\boldsymbol{Z}^p) \, , \tag{11}$$

where $\phi^i_{\boldsymbol{\alpha}^i}(\boldsymbol{Z}^i)$ is a polynomial basis in $\mathbb{R}^{m_i} \times \mathbb{R}^N$ and $\boldsymbol{\alpha}^i \in \mathbb{N}^{m_i}$ is a multi-index. Only if the components of each $\boldsymbol{Z}^i$ are statistically independent does this basis become a product of bases on $\mathbb{R} \times \mathbb{R}^N$. In general, a normalization factor has to be introduced to account for the joint measure on $\mathbb{R}^{m_i}$ (Soize and Ghanem, 2004). It should be noted that in the limit of infinite dimensional random variables $\boldsymbol{Z}^i$, the present construction does not necessarily hold and some additional compatibility conditions must be satisfied (Friedrichs, 1957). It is moreover noted that in the case of a chaos representation being fitted to observations, the formal representation of the random variables representing the parameters is not known (i.e. the functional form $\boldsymbol{f}(.)$ and the probability measure of the underlying random variables $\boldsymbol{Z}^i$ are not known). In this case, the Wiener chaos still provides a mean-square convergent representation in terms of multi-dimensional Hermite polynomials. The dimensionality of this representation should theoretically be infinite (expansions in terms of path of the Brownian motion and not just in terms of independent random variables), but can be expected to be finite and dependent on the scales of relevance in the problem (i.e. the infinite-dimensional behavior is a reflection of the quantum scale being significant).

In light of the above, only Gaussian measures will be used, and the development will serve as a template for other types of chaos. In this case, therefore, the basis functions are the multidimensional Hermite polynomials in independent Gaussian variables ($\boldsymbol{W}$), with $\boldsymbol{W} \in \mathbb{R}^v$, and the chaos expansion of a random vector $\boldsymbol{Y}$ will be expressed, for convenience, as

$$\boldsymbol{Y} = \sum_{j=0}^{P} \boldsymbol{y}_j \psi_j \quad \boldsymbol{Y}, \boldsymbol{y}_j \in \mathbb{R}^N \tag{12}$$

The symbols $\{\psi_i\}$ refer to polynomials in $\boldsymbol{W}$ which are orthogonal in the sense that their inner product $\langle \psi_j, \psi_k \rangle$, which is defined as the mathematical expectation of their product, evaluates to δ_{jk}. A complete probabilistic characterization of the process $\boldsymbol{Y}$ is obtained once the deterministic coefficients $\boldsymbol{u}_j$ have been calculated.

Recent efforts have been devoted to generalizing the polynomial chaos by relying on polynomials orthogonal with respect to other measures besides the Gaussian one (Babuska and Chantzipantelidis, 200; Xiu and Karniadakis, 2203; LeMaitre et.al, 2004a, 2004b). It should be noted that generalizing these representations beyond the Gaussian measure is a very delicate issue that could potentially violate the compatibility conditions associated with jointly distributed random variables, specially when infinite-dimensional random variables are involved (Friedrichs and Shapiro, 1957; Skorohod, 1974; Soize and Ghanem, 2004). The polynomial chaos built around the Gaussian measure (so-called Wiener-Hermite chaos) will be used in the present effort. It is emphasized here that this does not imply that the uncertainty in the governing equation is modeled as a Gaussian variable or process, it simply means that all uncertainties in the system, be they associated with physical parameters or solution processes, can be related to a reference Gaussian vector through a nonlinear transformation.

Estimation of Chaos Decompositions from Measurements

An essential ingredient in constructing a probabilistic model is the ability to suitably identify its parameters, In the present context, this is translated to the estimation of chaos representations from experimental observations. These observations can either be the data itself or some parameters obtained from the data through an inverse analysis. This could, for instance, be the case when material parameters are estimated from observations of the deformation of the material.

Four approaches have been pursued in this context. The first one relies on Maximum-Likelihood estimation (Descelliers et.al, 2005). The second relies on the Hilbert space structure afforded by the polynomial chaos construction (Sakamoto and Ghanem, 2002), and will estimate the coefficients through a least squares algorithm. The third approach develops a Bayesian inference framework in which to update prior estimates of the coefficients as measurements are obtained, and the fourth approach relies on Maximum Entropy formalism to construct estimates of the Chaos coefficients.

In addition to constructing an estimate of the parameters of the mathematical probabilistic model, the above procedures are also used to construct probabilistic models of the sampling distribution of these parameters. These sampling distributions are useful for determining the significance of additional experimental observations, (ε_d above, on the accuracy of the prediction. This will be briefly explained next.

The first step in the estimation procedures is to represent a stochastic process by its truncated Karhunen-Loeve approximation. Thus, for estimation purposes, a stochastic processes is identified by the joint probability measure of the Karhunen-Loeve variables, and of course, the eigenvalues and eigenvectors of its covariance kernel. As mentioned above, the case of random variables reduced trivially to a single term in the KL expansion.

Keeping in mind the ultimate objective, which is to construct a Polynomial Chaos representation of the stochastic process, the second step in the estimation task, then, consists of constructing the joint measure of the Karhunen-Loeve

variables. This can be done in a number of ways, depending on the procedure being adopted for the identification. For example, using the Maximum-Likelihood procedure or the Bayesian inference approach, there is no need to explicitly construct this probability measure. Rather, a algorithmic mapping from the KL-random variables to their probability measure is needed and can be readily developed through statistical sampling or a Markov Chain Monte Carlo (MCMC) procedure (Ghanem and Doostan, 2006). Using a Maximum entropy approach, on the other hand, an explicit expression can be obtained for the joint probability measure of the KL random variables.

Once the probability measures of the KL variables has been computed, a procedure is needed to construct the polynomial chaos coefficients for the underlying stochastic process. Again, using the Maximum Likelihood approach, this is done most easily by maximizing the likelihood function (Descelliers, Soize and Ghanem, 2004), using a numerical optimization approach. If an analytical expression is available for the KL variables, as is the case when the Maximum Entropy algorithm is used (Das and Ghanem, 2006), then a Rosenblatt transformation can be used to map the KL variables into a set of Gaussian variables. A polynomial approximation of this transformation is then readily constructed numerically. Clearly, should the KL variables be assumed to be independent, then a Nataf transformation is more expedient than the Rosenblatt one.

In all the above cases, an asymptotic sampling distribution of the polynomial chaos is obtained as a joint Gaussian measure with covariance obtained from the Fisher Information matrix of the estimated coefficients. This information is used to extend the original probabilistic mode, using polynomial chaos representations, by adding one more random variables to the set of independent random variables with respect to which the chaos is being developed. This new random variables, whose dimension is equal to the chaos parameters being estimated, represents the uncertainty in the model due to scarce data. Procedures for propagating this uncertainty to the model-based predictions are then identical to the procedures used for propagating the more standard uncertainty, associated with model parameter variability, as described next.

It is wort noting here that according to polynomial chaos theory, any L_2 functional of the brownian motion can be represented as an infinite-dimensional polynomial in gaussian variables. Any such functional, when represented in a finite-dimensional representation, will have its coefficients be function of all remaining variables (Slud, 1993). Of course, it may happen that the parameters being estimated do indeed belong to a finite-dimensional space, described by a finite number of gaussian random variables. This finite-dimensional property will manifest itself in the limit as infinitely many data points are used in estimating the coefficients, assuming that a polynomial chaos of sufficient dimensionality is used. In this case, the sampling distribution of the chaos coefficients will tend to a delta function around the true deterministic value.

The next section will review procedures for propagating the polynomial chaos representations, which capture both aleatory and epistemic uncertainty, through a predictive model, usually based on mechanics.

STOCHASTIC GOVERNING EQUATIONS AND PROPAGATION OF UNCERTAINTY

Two procedures for estimating the polynomial chaos coefficients of the solution, governed by the fundamental conservation laws, given a probabilistic description of system parameters, have been pursued in the literature. The first approach involves projecting the error in the governing equations onto the polynomial chaos basis while the second approach consists of projecting the error in the solution itself, onto that basis. The first approach requires significant access to the database of an analysis code and is thus labeled "intrusive", while the second approach requires minimal access to such databases and is thus labeled "non-intrusive".

Intrusive Approach: Minimizing the error in the governing equation

Without loss of generality, it will be assumed throughout that spatial discretization is achieved through a finite element procedure. Applying the finite element method to a physical problem governed by an equilibrium, evolution, or conservation law, reduces the problem to the solution of an N-dimensional algebraic system of equations of the form,

$$\boldsymbol{K}(\boldsymbol{u},\boldsymbol{a}(\theta))\boldsymbol{u}(\theta) \;=\; \boldsymbol{f}(\theta) \qquad \boldsymbol{u},\boldsymbol{f} \in \mathbb{R}^N \tag{13}$$

The random character of the model parameter $\boldsymbol{a}$ is made explicit by its argument θ. The possibility of some nonlinear dependence of $\boldsymbol{K}$ on the state of the system $\boldsymbol{u}$ is also made explicit. Representing the parameter $\boldsymbol{a}(\theta)$ in its polynomial chaos decomposition yields,

$$\boldsymbol{a}(\theta) = \sum_{i=0}^{L} \boldsymbol{a}_i \psi_i(\theta) \; . \tag{14}$$

Note that the algebraic character of random parameter $\boldsymbol{a}(\theta)$ (scalar, vector, tensor) depends on the particular model being treated. Following the traditional FE-assembly procedure, this leads to the corresponding expansion of the stiffness matrix,

$$\boldsymbol{K} = \sum_{i=0}^{L} \psi_i \boldsymbol{K}_i, \tag{15}$$

where $\boldsymbol{K}_0$ denotes the stiffness matrix for the mean material property and the other terms correspond to the random fluctuations about the mean. The coefficients $\boldsymbol{K}_i$ can be obtained as

$$\boldsymbol{K}_i = \frac{\langle \boldsymbol{K}\psi_i \rangle}{\langle \psi_i^2 \rangle} \ , \tag{16}$$

where the numerator is evaluated either analytically or by statistical sampling, depending on whether the dependence of the stiffness matrix on the random parameters is simple or not. The angled brackets, here, denote the operator of mathematical expectation. Expanding the solution with respect to the polynomial chaos basis,

$$\boldsymbol{u} = \sum_{j=0}^{P} \boldsymbol{u}_j \psi_j(\theta) \ , \quad \boldsymbol{u}, \boldsymbol{u}_j \in \mathbb{R}^N, \tag{17}$$

and substituting the expressions (15) and (17) into eq. (13), results in,

$$\sum_{j=0}^{P} \sum_{i=0}^{L} \psi_i \psi_j \boldsymbol{K}_i \boldsymbol{u}_j \ = \ \boldsymbol{f}(\theta) \ . \tag{18}$$

Equality in this last equation can be construed to be in the weak sense, namely as an equality of the respective projections of the left hand side and right hand side on sequence of finite-dimensional subspaces. This weak sense equality can be achieved by projecting the equation on the subspace spanned by the polynomial chaos subset used in the approximation. Recalling that the inner product on the Hilbert space of random variables is equivalent to the operation of linear correlation, this process results in the following equations,

$$\sum_{j=0}^{P} \sum_{i=0}^{L} \langle \psi_i \psi_j \psi_k \rangle \boldsymbol{K}_i \boldsymbol{u}_j \ = \ \langle \psi_k \boldsymbol{f}(\theta) \rangle \quad k = 0, 1, \ldots P \, . \tag{19}$$

This last equation can be rewritten as,

$$\sum_{j=0}^{P} \sum_{i=0}^{L} c_{ijk} \boldsymbol{K}_i \boldsymbol{u}_j = \boldsymbol{f}_k \quad k = 0, 1, \ldots P \, , \tag{20}$$

where the coefficients c_{ijk} denote $\langle \psi_i \psi_j \psi_k \rangle$ and $\boldsymbol{f}_k$ denotes $\langle \psi_k \boldsymbol{f}(\theta) \rangle$. This system of linear equations is to be solved for the unknown coefficients, $\boldsymbol{u}_j$, of the polynomial chaos expansion (Ghanem and Spanos, 1991). Implementation issues including applications to nonlinear and unsteady problems are addressed in a number of references (Ghanem and Dham, 1998; Ghanem and Red-Horse, 1999; Debusschere et.al 2004; Reagan et.al, 2005).

In case the random parameters appear as multiplicative coefficients in the governing equation, matrix $\boldsymbol{K}_i$ appearing in the above equation is obtained through a standard finite element assembly procedure with the material property throughout the domain replaced by the i^{th} polynomial chaos mode shape. For the case where the dependence on the parameters is more complex, either a Taylor expansion of this dependence, or statistical sampling procedures have been used to represent the random parameter (Ghanem and Dham, 1998).

Non-intrusive approach: Minimizing the error in the solution

The polynomial chaos coefficients of the solution vector $\boldsymbol{u}$ can be also estimated according to a procedure that does not require any modifications to the source code of an analysis software. This procedure relies on the representation of these polynomial chaos coefficients as generalized Fourier coefficients which can be obtained as the projection of the solution vector, $\boldsymbol{u}$, on the respective polynomial chaos basis functions. This results in the expression,

$$\boldsymbol{u}_i = \frac{\langle \boldsymbol{u}\psi_i \rangle}{\langle \psi_i^2 \rangle} \ . \tag{21}$$

The numerator in the above expression can be evaluated using statistical sampling. The convergence of the solution estimated according to this approach is sensitive to the number of statistical samples used in estimating the projection in the numerator.

EXAMPLES

Two examples will be described that demonstrate the modeling possibilities afforded by the methodology presented above.

Modeling and Propagation of Epistemic Uncertainty

In a first example, we extend a method developed to address limited statistical information (Red-Horse, 2004) to accommodate the effects of approximate information acquired from experimental information used to model a random field. The essential ingredient of this example is to recognize that any random quantity that we care about, no matter how ill-constrained it is by a certain physical set-up, can be characterized by its coordinates with respect to the polynomial chaos. The task then is to find these coefficients. In this first example, these coefficients are estimated through a search algorithm, and the uncertainty propagation problem is carried out using the non-intrusive approach described above.

The experimental information are represented by a correlation matrix with entries that correspond to physical points on a given structural domain.

These points are a small subset of the nodes available in a corresponding finite element model, and the entries in the correlation matrix are given as intervals reflecting the limited number of samples used in estimating it.

Our process begins by generating 100 covariance matrices satisfying the joint bound constraints present in the experimentally-estimated correlation matrix. Care is taken to ensure the positivity and symmetry of each of these 100 matrices. While symmetry can be readily imposed, positivity is achieved by enforcing the positivity of the eigenvalues of the correlation matrix.

Next we construct a Karhunen-Loève (KL) expansion (Ghanem and Spanos, 1991) for each covariance matrix, and build a family of random fields by representing each KL random variable as a polynomial chaos expansion (PCE) (Ghanem and Spanos, 1991) and testing to ensure that a given field continues to satisfy aforementioned statistical constraints. The KL variables represent the discretization of the stochastic field into a denumerable set of random variables, and they encapsulate the complete probabilistic character of the field. These KL random variables, which are typically statistically dependent, are completely characterized by their joint probability measure, which is furthermore usually non-Gaussian. While the non-Gaussian property if maintained in our present work, the assumption of independence is made to simplify the exposition. To provide a computationally tractable representation of the non-Gaussian vector appearing in the KL expansion, this vector is approximated by a finite length Polynomial Chaos (PC) expansion. Generally, this is an expansion of a stochastic process as a multidimensional polynomial in independent Gaussian random variables (Ghanem and Spanos, 1991). A tenth order, one-dimensional approximation is used for each of the KL variables.

The KL representation expresses the random fields as a series of deterministic shapes with random amplitudes. The deterministic shapes inherit the functional properties of the data from which the process is being synthesized. In our present work, we are interested in situations where the data is observed sparingly over the spatial domain of definition of the process, thus requiring an interpolation process to complete the characterization of the random field. We achieve this by utilizing radial basis functions (Buhmann, 2003) to expand from the data observation points to all of the nodes in the domain of the random field.

For each field in the set of analytical random fields that cannot be rejected based on the available information, we propagate the uncertainty to the system response using stochastic finite element techniques, with the response represented as a PCE with Fourier coefficients computed using a numerical cubature technique (Genz, 1996). Thus, the KL variables are sampled at the cubature coordinates, the deterministic problem associated with each of these samples is solved using an analysis tool (in this case finite elements) as a black box, and the multi-dimensional Hermite polynomial representation of the solution constructed through statistical averaging.

The specific application of interest here involves an epoxy foam with spatially varying stiffness properties that, through the mixing and pouring process, are known to vary sample to sample. The top part of Figure (1) shows the foam material the elasticity of which is assumed to have been observed at 30 spatial locations scattered on its surface. The bottom part of Figure (1) shows the probability density functions of the maximum acceleration. It is emphasized that all the probability density functions shown in this figure are consistent with the limited available information. The scatter in these curves can be used as an indication as to the suitability of the experimental effort and its sufficiency towards a validation exercise.

Propagation of Epistemic Uncertainty

As a second example, highlights the intrusive approach and demonstrates the propagation of the sampling error component to the model-based prediction. This in turn permits the determination as to whether additional data points are needed to better characterize the confidence in the prediction. Consider the following one-dimensional problem,

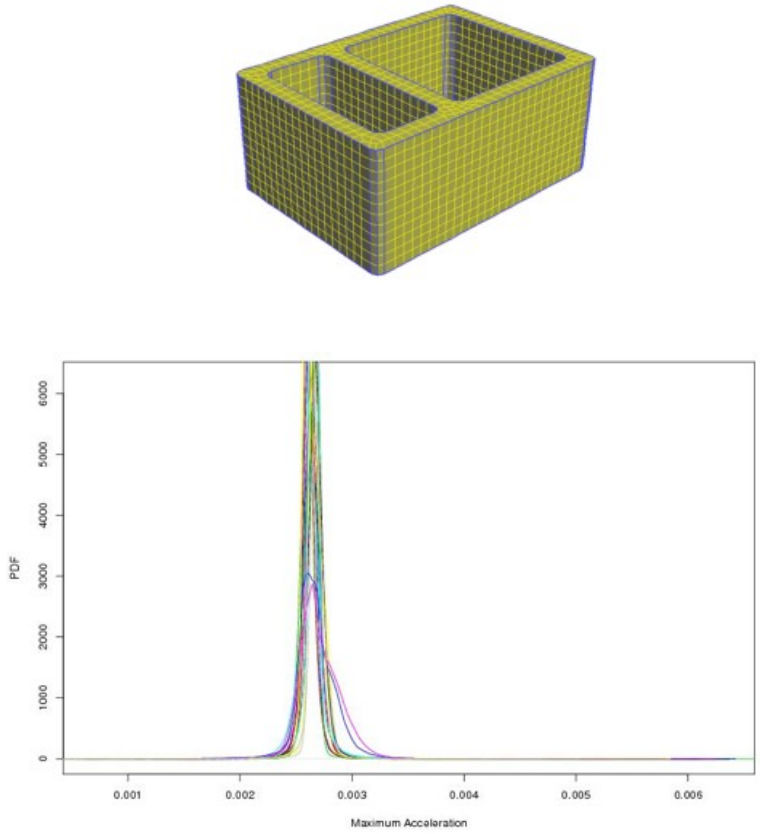

Figure 1 – Top: Foam material; Bottom: Probability Density Functions for Maximum Acceleration.

$$\begin{aligned} -\frac{\mathrm{d}^2 u(x,\omega)}{\mathrm{d}x^2} &= a(x,\omega) \quad x \in \mathscr{D} = (-0.5,+0.5) \\ u(\pm 0.5,\omega) &= 0, \end{aligned} \tag{22}$$

where $a(x,\omega)$ is the underlying input function for which observations are available on the set $\Xi = \{-0.5,-0.25,0,0.25,0.5\}$. A random field with known probabilistic structure for a is used to generate a limited number of realizations of the process on a set of observation points, Ξ, inside $\mathscr{D}$. It is assumed that the dominant eigenspace of the associated covariance matrix of the observations as well as the mean of the observations are close enough to the corresponding exact values. The only other inputs to the algorithm is the recorded data along with the geometry of the domain. After estimating the unknown parameters, the marginal distribution of the original process and those of the reconstructed one are compared. Furthermore the variability of the parameter estimates are propagated to the response of (22) and the effect of such variability on the statistics of the solution can then be analyzed.

Figure (2) shows the probability density function of the solution, evaluated at $x = 0$, for different number of observations (M) used in the probabilistic calibration. In each of the four plots shown in the Figure, the error bars indicate the 95% confidence intervals consistent with the sampling distribution of the error stemming from the small data assumption. As expected, these error bars reduce in width as the number of observations is increased. It is noted that the probability density functions shown in this figure are obtained from the computed polynomial chaos expansion by synthesizing a large number of realizations of the stochastic solution and constructing a probability density function from the resulting statistical sample. Kernel density estimation techniques are used to that end.

CONCLUSION

A careful observation of the above results highlights the significance of adaptivity with respect to the number of experimental data points used in calibrating the stochastic system parameters. More specifically, both the estimates and the associated statistical confidence are affected by the experimental sample size used in the estimation algorithm, and the accuracy of both quantities increases with more observations. This parallels the concept of error analysis in the finite element solution of deterministic partial differential equations where both the approximate solution and the associated a posteriori error estimates are obtained more accurately as the descritization spaces are enriched. It is noted that this

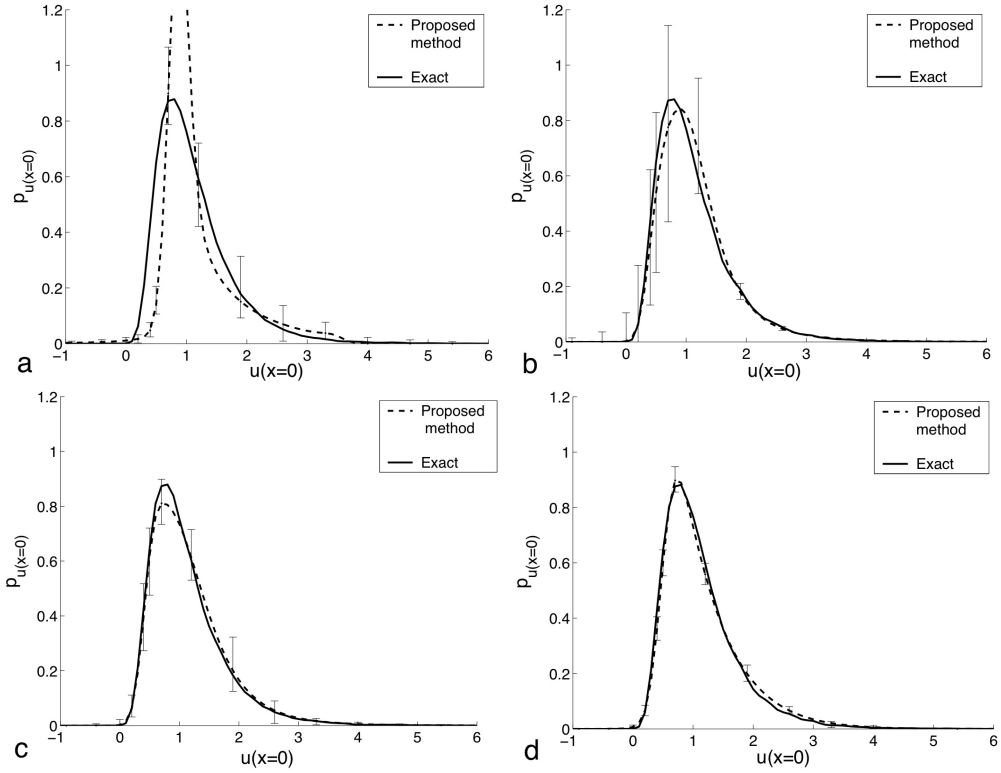

Figure 2 – Probability density function of $u(x=0)$ with 95 percent confidence intervals around the estimated density. (a) $M=20$. (b) $M=30$. (c) $M=50$. (d) $M=100$. (M=number of samples used in calibration.

parallelization between the deterministic and the stochastic cases is greatly facilitated by the product space constructions and associated projections adopted in conjunction with the polynomial chaos decompositions.

ACKNOWLEDGMENT

Financial support from various sources including NSF, AFOSR, ONR, DARPA and Sandia is gratefully acknowledged. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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