8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

CONTRASTS AND CONNECTIONS BETWEEN COMPUTATIONAL METHODS FOR SPDES

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Key Words: *polynomial chaos methods, stochastic collocation methods, stochastic sampling methods, stochastic PDEs*

ABSTRACT

Physical, biological, social, economic, financial, etc. processes always involve uncertainties. *Uncertainty quantification* is the task of determining statistical information about outputs of a system or process, given statistical information about the inputs. Here, we are interested in systems for which solutions of a partial differential equation (PDE) are used to define the mapping from the input variables to the output variables. Accounting for uncertainty in processes governed by PDEs can involve input data in the form of random coefficients and right-hand sides in the PDEs, boundary conditions, and initial conditions and even random geometries, i.e., random boundary shapes. Uncertainty arises because available data are incomplete or unpredictable. In the former case, the data may be predictable but are too difficult (perhaps even impossible) or costly to obtain by measurement. Uncertainty can also arise because not all scales in the data and/or solutions can or should be resolved or because some scales may not be of interest. In the former case, it may be too difficult (perhaps impossible) or costly to do so in a computational simulation.

Here, we are interested in stochastic PDE (SPDE) problems whose definition involves a finite number which is independent of the spatial grid size, of random parameters. The parameters may be settings that define the input data, e.g., “knobs” in an experiment, or may result from, e.g., Karhunen-Loevy, approximations of correlated random fields.

Each parameter y_n, $n = 1, \ldots, N$, could be distributed independently according to a corresponding probability density function (PDF) $\rho_n(y_n)$, each of which is a mapping from a possibly infinite interval $\mathcal{I}_n$ into the real numbers. Alternately, the parameters could be distributed according to a joint PDF $\rho(y_1, \ldots, y_N)$ that is a mapping from an N-dimensional set Γ into the real numbers. Independently distributed parameters are the special case for which

$$\rho(y_1, \ldots, y_N) = \prod_{n=1}^{N} \rho_n(y_n) \qquad \text{and} \qquad \Gamma = \mathcal{I}_1 \otimes \mathcal{I}_2 \otimes \cdots \otimes \mathcal{I}_N$$

in which case, after simple rescalings, Γ is a (possibly infinite) hypercube in $\Re^N$.

To provide a concrete context for our discussions, we consider a specific class of problems. Let $\mathcal{D} \subset \Re^d$, $d = 1, 2$, or 3, denote a spatial domain and let $\Gamma \in \Re^N$ denote a parameter domain, where N denotes the number of parameters. We have that $\mathbf{x} \in \mathcal{D}$ denotes the spatial variable and $\vec{y} = (y_1, y_2, \ldots, y_N) \in \Gamma$ the parameter vector. For appropriate spaces X and Z, we then seek $u \in X \times Z$ such that

$$\int_\Gamma \int_\mathcal{D} S(u; \vec{y}) T(v) \rho(\vec{y})\, d\mathbf{x} d\vec{y} = \int_\Gamma \int_\mathcal{D} v f(\vec{y}) \rho(\vec{y})\, d\mathbf{x} d\vec{y} \qquad \forall\, v \in X \times Z, \tag{1}$$

where $S(\cdot;\cdot)$ is, in general, a nonlinear operator and $T(\cdot)$ is a linear operator, both possibly involving derivatives with respect to $\mathbf{x}$; these can also depend on $\mathbf{x}$ but, to avoid unnecessary notational complexities, we do not explicitly keep track of such dependences.Also for the sake of simplicity, we consider stationary problems; all we have to say holds equally well for time-dependent problems.

A *realization* $u(\mathbf{x}; \vec{y})$ of a solution of an SPDE is a solution of the deterministic PDE obtained for a specific choice of the random parameters$\{y_n\}_{n=1}^N$. In general, there is no interest in individual realizations. One may be interested in *statistical information* about solutions of the SPDE such as the average or expected value, the covariance, the variance, higher moments, or even their whole PDF. However, quantities obtained by post-processing solutions of the SPDE are often of even greater interest. Of course, one still has to solve the SPDE to determine the quantity of interest.

Again for the sake of concreteness, here we focus on the very useful class of *quantities of interest* that involve integrals over the parameter space, e.g., integrals of the type

$$\int_\Gamma G\big(u(\mathbf{x}; \vec{y})\big) \rho(\vec{y})\, d\vec{y} \qquad \text{or possibly} \qquad \int_\Gamma G\big(u(\mathbf{x}; \vec{y}); \mathbf{x}, \vec{y}\big) \rho(\vec{y})\, d\vec{y}$$

for some $G(\cdot)$. Integrals of these types cannot, in general, be evaluated exactly. Thus, they are approximated using a quadrature rule

$$\int_\Gamma G\big(u(\mathbf{x}; \vec{y})\big) \rho(\vec{y})\, d\vec{y} \approx \sum_{q=1}^{Q} w_q \rho(\vec{y}_q) G\big(u(\mathbf{x}; \vec{y}_q)\big) \tag{2}$$

for some choice of quadrature weights $\{w_q\}_{q=1}^Q$ (real numbers) and quadrature points $\{\vec{y}_q\}_{q=1}^Q$ (points in the parameter domain Γ.) Alternately, the probability density function is sometimes used in the determination of the quadrature points and weights so that instead one ends up with an approximation of the form

$$\int_\Gamma G\big(u(\mathbf{x}; \vec{y})\big) \rho(\vec{y})\, d\vec{y} \approx \sum_{q=1}^{Q} w_q G\big(u(\mathbf{x}; \vec{y}_q)\big).$$

Again, to provide a concrete context, we assume that all methods we consider use the same approach to effect discretization with respect to the spatial variables and that that approach is based on finite element methods. Sometime such methods are referred to, in the context of SPDEs, as *stochastic finite element methods.*

Using the context provided by SPDEs of the form (1) and approximations of quantities of interest of the form (2), we review, compare, and contrast several popular methods for determining output quantities of interest that depend on solutions of SPDEs. The main objective is to explore the connections between the different methods. In particular, we will show how all these methods can be put into a single framework, i.e., they are all special cases of *stochastic Galerkin methods.* This is not merely a mathematical nicety; placing the methods within a single framework facilitates making connections between them and comparing their relative merits. The discussion includes, but is not limited to, intrusive and non-intrusive polynomial chaos, stochastic collocation, and stochastic sampling methods