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Uncertainty Quantification (UQ)

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Uncertainty Quantification (UQ) is an emerging field in computational engineering that can provide certificates of fidelity in a simulation beyond the standard numerical error, and it includes uncertainty in boundary conditions, constitutive laws, materials properties and geometries. UQ is particularly impornat at microscales where geometric roughness and material properties cannot be readily quantified experimentally. Here we present a general framework for UQ based on the generalized polynomial chaos approach and various extensions that do not require modification of existing codes and are particularly effective in Microsystems with many uncertain parameters (e.g. high dimensionality).

UQ requires the propagation of uncertainty through a given mathematical model and affects all stages of numerical simulation. Specifically, partial differential equations widely used to formulate mathematical models of physical systems must be reformulated as stochastic partial differential equations, posing new challenges for mathematics (pure and applied alike), parsimonious parametric description of stochastic input data and model calibration requires methods from statistics, and the numerical solution of stochastic partial differential equations will equally impact numerical analysis and scientific computing.

In practical applications, at most second-order expansions are employed -- the so-called '*first order - second moment analysis*' [1] that has been used extensively in engineering applications. An inherent limitation of such first order perturbation methods is that the uncertainties must not be too large, i.e., the fluctuations of the random fields should be small compared to their mean values (typically less then 10%). This requirement needs to be satisfied not only by the stochastic inputs but also by the stochastic outputs; this is especially difficult to verify *a priori* for nonlinear problems, as small fluctuations in random inputs may result in large fluctuations in the systems' responses. Also, higher-order statistics of input data are not readily available. A related approach is based on manipulation of the stochastic operators. Methods include the Neumann expansion, which is based on expanding the inverse of the stochastic operator in a Neumann series [2], and the weighted integral method [3]. These methods have limitations on the type of model equations they can address, and, if truncated after second moment terms, are also restricted to small uncertainties. Here, we review an efficient approach for the deterministic approximation of second and higher order spatial correlations of random solutions, based on polynomial chaos expansion, where the "stochasticity" in the solution is transferred in the trial basis and hence one solves for appropriate PDEs for the deterministic coefficients of the polynomial chaos expansion.

Ghanem and Spanos in [4] pioneered the computational use of the *polynomial chaos* (PC) expansion method, and have successfully applied it to various problems in solid mechanics. PC expansions are based on the homogeneous chaos theory of N. Wiener and are essentially spectral expansions of Gaussian random fields into Hermite Polynomials. PC expansions allow high-order deterministic approximation of random fields and appear to exhibit spectral convergence in many cases as we will show. Classical Wiener-Hermite PC expansions are based on the *Hermite* polynomial functionals in terms of *Gaussian* random variables. In theory, they converge to any L_2 functional on the random space. However, in practice they converge slowly for non-Gaussian random fields and do not apply to random fields with *discrete* distributions. Accordingly, for fast convergence in PC expansions and, hence, for computational efficiency, the "coordinates in probability space" in which PC expansions of the random solution are sought should be adapted to the statistics of the input data and of the random solution. Galerkin projection can be employed to obtain the deterministic system of equations, and this has been done in various engineering systems.

In generalized polynomial chaos (gPC), the polynomials are chosen from the hypergeometric polynomials of the *Askey family*, where the underlying random variables are not restricted to Gaussian random variables. In fact, there exists a unique correspondence between the probability distribution function (PDF) of the stochastic input and the weighting function of the orthogonal polynomials. The convergence properties of different trial bases were studied in [5] and exponential convergence rate was demonstrated computationally for model problems. The aforementioned correspondence can be extended to arbitrary PDFs with the orthogonal polynomials constructed *on-the-fly*; this extension was presented in [6]. For nonlinear operators, gPC with Galerkin projection may not be efficient because of the resulted undesirable complexity. Recently, collocation projection of gPC method, based on *sparse grids*, has received considerable attention due to its simplicity and efficiency in

dealing with nonlinear operators. Depending on the stochastic regularity in the parametric space, it can be advantageous to combine mesh refinement with increase of the polynomial degree, leading to an *hp-generalization* of gPC approximations, see [7]. There exist various ways to construct local polynomial chaos basis, such as piecewise polynomials in [8] and wavelets in [9]. The multi-elment generalized polynomial chaos (ME-gPC) was developed in [7], where local orthogonal basis is constructed numerically according to the local conditional PDF.

For a general (nonlinear) operator, a Galerkin projection on the polynomial chaos basis can result in a highly coupled PDE system, which may not be easy to solve numerically. To enhance the efficiency of polynomial chaos methods without a sacrificing accuracy, we can consider the collocation projection. The key of collocation projection is how to choose the grid points in the parametric multi-dimensional space. Obviously, full tensor-products of one-dimensional grid points are not proper due to the "curse of dimensionality". So far, much attention has been paid on the sparse grids because of its weak dependence on dimensionality. In figure 1, we compare the patterns of full tensor-product grids and nested sparse grids.

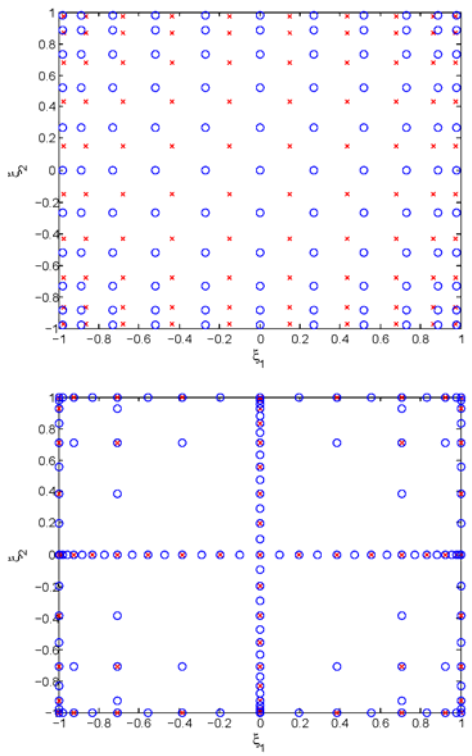

Figure 1. Patterns of full tensor-product grids (upper) and sparse grids (lower). '×' and 'o' indicate grid points at two subsequent levels.

Several examples from fluids and heat transfer will be presented demonstrating some of the advantages of stochastic modelling of Microsystems, including global sensitivity analysis, which is a natural by-product of the PC formalism. The most effective approach for high-dimensional parametric uncertainties is the multi-element probabilistic collocation method combined with ANOVA, see [10].

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