

Efficient Solution of Ordinary Differential Equations with High-Dimensional Parametrized Uncertainty

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Abstract. The important task of evaluating the impact of random parameters on the output of stochastic ordinary differential equations (SODE) can be computationally very demanding, in particular for problems with a high-dimensional parameter space. In this work we consider this problem in some detail and demonstrate that by combining several techniques one can dramatically reduce the overall cost without impacting the predictive accuracy of the output of interests. We discuss how the combination of ANOVA expansions, different sparse grid techniques, and the total sensitivity index (TSI) as a pre-selective mechanism enables the modeling of problems with hundred of parameters. We demonstrate the accuracy and efficiency of this approach on a number of challenging test cases drawn from engineering and science.

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1 Introduction

Quantifying the impact of uncertainty in physical systems has received considerable attention during the last decade, in particular emphasizing the need to develop efficient and accurate computational techniques for high-dimensional problems. Applications of such techniques can be found across the sciences and engineering with the uncertainty being caused by insufficient or inaccessible data among other things.

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In this work we consider problems of the type

$$\begin{aligned}\frac{d\mathbf{u}(t,\boldsymbol{\alpha})}{dt} &= \mathbf{f}(\mathbf{u},t,\boldsymbol{\alpha}), \quad t > 0, \\ \mathbf{u}(0,\boldsymbol{\alpha}) &= \mathbf{g}(\boldsymbol{\alpha}),\end{aligned}$$

where the state vector $\mathbf{u} : \mathbb{R}^+ \times \mathbb{R}^p \rightarrow \mathbb{R}^m$, and the flux $\mathbf{f} : \mathbb{R}^m \times \mathbb{R}^+ \times \mathbb{R}^p \rightarrow \mathbb{R}^m$ is assumed Lipschitz continuous. The solution is parameterized by $\boldsymbol{\alpha} = (\alpha^1, \dots, \alpha^p)$ which describes the system, e.g., the details of the initial conditions or parameters in the flux.

This very general problem arises in numerous applications and there is a long history of the development of accurate and efficient methods for solving them provided $\boldsymbol{\alpha}$ is known accurately. We think of this as the purely deterministic case. However, for many problems, the parameters are not known, known only with poor accuracy, or even entirely inaccessible. One approach in such cases is to endow the parameters with a confidence interval and associated probability density, hence turning the problem into a stochastic problem. We must then consider methods that enable the rapid computation of statistical measures such as the mean and variances of the state variables. This clearly has to be approached carefully since minor, but correlated, changes in some parameters may lead to major changes in the output variables. Simply freezing the parameters at expectation values is generally far from adequate.

It is reasonable to categorize the majority of methods for computationally dealing with such problems into two groups: sampling based statistical methods and probabilistic techniques. In the first category one finds the classic Monte Carlo (MC) method [5] which has the clear advantage of being simple, e.g., one needs only a deterministic solver. The simplicity, however, comes at the cost of slow convergence as $\mathcal{O}(K^{-1/2})$ where K is the number of samples. This quickly becomes prohibitive if even reasonable accuracy is needed, in particular if the interest is on higher moments such as variance/sensitivity. To accelerate convergence of the MC method, several techniques have been proposed, e.g., Latin hypercube sampling [24], quasi-MC (QMC) method [6], and the Markov chain MC (MCMC) [7] method. However, additional restrictions are often imposed by these methods and their applicability is not general.

A particular alternative to sampling based techniques has recently received substantial attention. Known as Stochastic Galerkin or Polynomial Chaos (PC) methods, these are probabilistic in nature and based on a generalization of the Wiener-Hermite PC expansion. In this approach, the randomness is represented by the Wiener expansion and the unknown expansion coefficients are found by a Galerkin procedure in the inner product associated with the measure of the random variables used in the Wiener expansion.

Substantial recent work has shown the accuracy and efficiency of this approach, in particular for problem of low to moderate dimensionality and problems with sufficient smoothness in probability space, enabling a very efficient representations through the Wiener expansion. However, a substantial disadvantage of the Galerkin approach is the need to develop entirely new software to solve large coupled equations resulting from