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Efficient Collocational Approach for Parametric Uncertainty Analysis

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Abstract. A numerical algorithm for effective incorporation of parametric uncertainty into mathematical models is presented. The uncertain parameters are modeled as random variables, and the governing equations are treated as stochastic. The solutions, or quantities of interests, are expressed as convergent series of orthogonal polynomial expansions in terms of the input random parameters. A high-order stochastic collocation method is employed to solve the solution statistics, and more importantly, to reconstruct the polynomial expansion. While retaining the high accuracy by polynomial expansion, the resulting "pseudo-spectral" type algorithm is straightforward to implement as it requires only repetitive deterministic simulations. An estimate on error bounded is presented, along with numerical examples for problems with relatively complicated forms of governing equations.

AMS subject classfications: 65C20, 65C30

Key words: Collocation methods, pseudo-spectral methods, stochastic inputs, random differential equations, uncertainty quantification.

1 Introduction

The focus of this paper is on efficient numerical methods for differential/algebraic equations with random/uncertain parameters. In the past years, this subject has received increasing amount of attention in a variety of engineering disciplines, especially those involving complex physics. In such complex fields, mathematical models can only serve as simplified and reduced representations of true physics, and there exists a significant amount of uncertainty associated with parameter values, boundary/initial conditions, constitutive laws, etc. For example, biochemical reactions are often modeled by (large) systems of ordinary differential equations (ODEs) or differential-algebraic equations (DAEs). Although these models have been successful in revealing quantitative connections between reaction details and observables, their usage is often constrained by the

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difficulty of assigning numerical values to kinetic parameters (e.g., rate constants and binding constants) in the governing equations. Common approach is to conduct parameter estimation, in order to bring numerical solutions in reasonable agreement with a set of experimental observations. Because of the complexity of most biochemical processes and the diversity of the type of data to be fitted, the estimated model parameters usually contain significant uncertainties, rather than having precise numerical values. Traditional approach assigns "most likely" values to the parameters from their corresponding ranges, and such an approach could be inadequate as the complex biochemical processes may depend sensitively to some of the parameters. Also, very often observables from experiment measurements are not repeated enough times for reliable statistical estimates to be made on the "likelihood" of the parameter values. (General discussions on mathematical biology can be found in [6, 21], etc.) Therefore, mathematical and numerical techniques are needed to develop effective means of quantifying parameter uncertainty and its effect in complex systems.

In this paper we discuss an efficient method for parametric uncertainty analysis in (ordinary) differential-algebraic equations (DAEs). The uncertain parameters associated with the models are modeled as random variables. Subsequently, the resulting DAEs become stochastic equations. We remark that this type of stochastic systems are different from the classical "stochastic differential equations" (SDE) where the random inputs are some idealized processes such as Wiener processes, Poisson processes, etc., and tools such as stochastic calculus have been developed extensively and are still under active research. (See, for example, [9, 14, 15, 20].) In the problems considered in this paper, the random inputs are parameters modeled as random variables.

One of the most commonly used methods is Monte Carlo sampling (MCS), or one of its variants. Although MCS is straightforward to apply as it only requires repetitive executions of deterministic simulations, typically a large number of such executions are needed as the solution statistics converge relatively slowly, e.g., the mean value typically converges as $1/\sqrt{K}$ where K is the number of realizations [7]. The resulting statistical errors due to insufficient number of realizations can undermine the conclusions of uncertainty analysis such as the level of confidence in model selection and parameter estimates, etc. The need for large number of realizations for accurate results can incur excessive computational burden, especially for systems that are already computationally intensive in their deterministic settings.

A recently developed method, generalized polynomial chaos (gPC) [28, 30], belong to the class of non-sampling methods. With gPC, stochastic quantities are expressed as orthogonal polynomials of the input random parameters, and different types of orthogonal polynomials can be chosen to achieve better convergence. gPC expansion is essentially a spectral representation in random space, and exhibits fast convergence when the expanded function depends smoothly on the random parameters. Exponentially fast convergence can be achieved under certain circumstances. (See [2,28] for detailed discussions.)

When applied to differential equations with random inputs, the quantities to be solved