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Mesh refinement for uncertainty quantification through model reduction

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ABSTRACT

We present a novel way of deciding when and where to refine a mesh in probability space in order to facilitate uncertainty quantification in the presence of discontinuities in random space. A discontinuity in random space makes the application of generalized polynomial chaos expansion techniques prohibitively expensive. The reason is that for discontinuous problems, the expansion converges very slowly. An alternative to using higher terms in the expansion is to divide the random space in smaller elements where a lower degree polynomial is adequate to describe the randomness. In general, the partition of the random space is a dynamic process since some areas of the random space, particularly around the discontinuity, need more refinement than others as time evolves. In the current work we propose a way to decide when and where to refine the random space mesh based on the use of a reduced model. The idea is that a good reduced model can monitor accurately, within a random space element, the cascade of activity to higher degree terms in the chaos expansion. In turn, this facilitates the efficient allocation of computational sources to the areas of random space where they are more needed. For the Kraichnan–Orszag system, the prototypical system to study discontinuities in random space, we present theoretical results which show why the proposed method is sound and numerical results which corroborate the theory.

1. Introduction

Generalized polynomial chaos (gPC) is a frequently used approach to represent uncertain quantities when solving differential equations involving uncertainty in initial conditions, boundary conditions, randomness in material parameters and etc. Based on the results of Wiener [1], spectral expansion employing Hermite orthogonal polynomials was introduced by Ghanem and Spanos [2] for various uncertainty quantification problems in mechanics. This method was generalized by Xiu and Karniadakis [3,4] to include other families of orthogonal polynomials. When the solution is sufficiently regular with respect to the random inputs, the gPC expansion has an exponential convergence rate [3]. However, if the solution is not smooth, the rate of convergence of gPC deteriorates similarly to the deterioration of a Fourier expansion of non-smooth functions [5]. The reason for the lack of smoothness can be, for example, the presence of certain values of the random input around which the solution may change qualitatively (this is called a discontinuity in random space). For such problems, the brute force approach of using more terms in the gPC expansion is prohibitively expensive.

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An alternative to using higher terms in the expansion is to divide the random space into smaller elements where a lower degree polynomial is adequate to describe the randomness [6]. This approach requires a criterion (a mechanism) to decide how to best partition the random space. Ideally, the criterion will focus on parts of random space, like discontinuities, where there is more sensitive dependence on the value of the random parameters. In addition to the presence of discontinuities in random space, there are problems which simply have too many sources of uncertainty to allow for a high degree expansion in all dimensions of random space. For some problems not all of the sources of uncertainty are equally important. This means that some directions in random space need more refinement than others. So, one needs to be able to identify correctly these directions and allocate accordingly the available computational resources.

In [7], one of the current authors proposed a novel algorithm for performing mesh refinement in *physical* space by using a reduced model. The algorithm is based on the observation that the need for mesh refinement is dictated by the cascade of energy (or mass depending on the physical context) to scales smaller than the ones resolved. A good reduced model should be able to effect with accuracy the necessary cascade of energy across scales. Thus, a good reduced model can be used to decide when to refine. In [7], a reduced model, called the t-model, which was derived through the Mori–Zwanzig formalism [8] was used to monitor the cascade of energy for partial differential equations that develop singularities. This particular model was constructed under the assumption that there is no timescale separation between the resolved and unresolved scales. This absence of timescale separation is an essential feature of problems which require mesh refinement. The solution exhibits small scale features that are important for the dynamic evolution of the solution at all scales.

In the current work we have used the same idea to aid with the task of mesh refinement in *random* space. In particular, we construct a reduced model for the system resulting from a gPC expansion of the random solution in each element of the random space (for the problems examined here we have also used the t-model as a reduced model). Then, this reduced model is used to monitor the cascade of energy from the resolved to the unresolved terms in the gPC expansion within an element.

What is needed to define a mesh refinement algorithm is a criterion to determine whether it is time to perform mesh refinement. In [7], this criterion was based on monitoring the contribution of memory term from reduced model to the rate of change of the L_2 norm of the solution at the resolved scales as computed by the reduced model (note that the L_2 norm corresponds to the mass or energy in many physical contexts). When this contribution value exceeds a prescribed tolerance the algorithm performs mesh refinement. In the current work we use the same criterion to decide if a random element needs to be refined. The suitability of the contribution of memory term to the rate of change of the L_2 norm as an indicator for the need to refine is shown in Appendix C. In particular, we show that in Kraichnan–Orszag system such contribution for the resolved scales has the same functional form as the expression for the rate of change of the L_2 error of the reduced model. Thus in this particular system, by keeping, through mesh refinement, the memory term contribution to the rate of change of the L_2 norm for the resolved scales under a prescribed tolerance, we can keep the error of the calculation under control (see Section 3 for more details).

The paper is organized as follows. In Section 2, we recall the framework for the stochastic Galerkin formulation of a random system. The proposed mesh refinement algorithm is presented in Section 3. Section 4 contains numerical results from the application of the algorithm. Conclusions are drawn in Section 5. Finally, in Appendix A we briefly state the Mori–Zwanzig formalism. Appendix B contains the Galerkin formulation of the Kraichnan–Orszag system as well as the reduced model used in the mesh refinement algorithm. Appendix C involves a proof of convergence of the reduced model.

2. gPC representation of uncertainty

Let $(\Omega, \mathcal{A}, \mathcal{P})$ be a probability space, where Ω is the event space and $\mathcal{P}$ is the probability measure defined on the σ-algebra of subsets of Ω. Let $\boldsymbol{\xi} = (\xi_1, \cdots, \xi_d)$ be a d-dimensional random vector for the random event $\omega \in \Omega$. Without loss of generality, consider an orthonormal generalized polynomial chaos basis $\{\Phi_{\mathbf{i}}\}_{|\mathbf{i}|=0}^{\infty}$ spanning the space of second-order random processes on this probability space ($\mathbf{i} = (i_1, \cdots, i_d) \in \mathbb{N}_0^d$ is a multi-index with $|\mathbf{i}| = i_1 + \cdots + i_d$). The basis functions $\Phi_{\mathbf{i}}(\boldsymbol{\xi}(\omega))$ are polynomials of degree $|\mathbf{i}|$ with orthonormal relation

$$\langle \Phi_{\mathbf{i}}, \Phi_{\mathbf{j}} \rangle = \delta_{\mathbf{ij}}, \tag{1}$$

where $\delta_{\mathbf{ij}}$ is the Kronecker delta and the inner product between two functions $f(\boldsymbol{\xi})$ and $g(\boldsymbol{\xi})$ is defined by

$$\big\langle f(\boldsymbol{\xi}), g(\boldsymbol{\xi}) \big\rangle = \int_{\Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) d\mathcal{P}(\boldsymbol{\xi}). \tag{2}$$

A general second-order random process $u(\omega) \in L_2(\Omega, \mathcal{A}, \mathcal{P})$ can be expressed by gPC as

$$u(\omega) = \sum_{|\mathbf{i}|=0}^{\infty} u_{\mathbf{i}} \Phi_{\mathbf{i}}\big(\boldsymbol{\xi}(\omega)\big). \tag{3}$$

The mean and variance of $u(\omega)$ can be expressed independently of the choice of basis as

$$\mathbb{E}\big(u(\boldsymbol{\xi})\big) = u_{\mathbf{0}}, \qquad \mathrm{Var}\big(u(\boldsymbol{\xi})\big) = \sum_{|\mathbf{i}|=1}^{\infty} u_{\mathbf{i}}^2, \tag{4}$$