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Doctoral Thesis

Advanced Methods in Stochastic Collocation for Polynomial Chaos in RAVEN

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Abstract

As experiment complexity in fields such as nuclear engineering continues to increase, so does the demand for robust computational methods to simulate them. In many simulations, input design parameters as well as intrinsic experiment properties are sources of input uncertainty. Often, small perturbations in uncertain parameters have significant impact on the experiment outcome. For instance, when considering nuclear fuel performance, small changes in the fuel thermal conductivity can greatly affect the maximum stress on the surrounding cladding. The difficulty of quantifying input uncertainty impact in such systems has grown with the complexity of the numerical models. Traditionally, uncertainty quantification has been approached using random sampling methods like Monte Carlo. For some models, the input parametric space and corresponding quantity-of-interest output space is sufficiently explored with a few low-cost computational calculations. For other models, it is computationally costly to obtain a good understanding of the output space.

To combat the costliness of random sampling, this research explores the possibilities of advanced methods in stochastic collocation for generalized polynomial chaos (SCgPC) as an alternative to traditional uncertainty quantification techniques such as Monte Carlo (MC) and Latin Hypercube sampling (LHS) methods. In this proposal we explore the behavior of traditional SCgPC construction strategies, as well as truncated polynomial spaces using total degree (TD) and hyperbolic cross (HC) construction strategies. We also consider applying anisotropy to the polynomial space, and analyze methods whereby the level of anisotropy can be approximated. We review and develop potential adaptive polynomial construction strategies. Finally, we add high-dimension model reduction (HDMR) expansions, using SCgPC representations for the constituent terms, and consider adaptive methods to construct them. We analyze these methods on a series of models of increasing complexity. We primarily use analytic methods of various means, and finally demonstrate on an engineering-scale neutron transport problem. For this analysis, we demonstrate the application of the algorithms discussed above in `raven`, a production-level uncertainty quantification framework.

Finally, we propose additional work in enhancing the current implementations of SCgPC and HDMR.

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Chapter 1

Introduction

In simulation modeling, we attempt to capture the behavior of a physical system by describing it in a series of equations, often partial differential equations. These equations may be time-dependent, and capture physics of interest for understanding the system. A *solver* is then written that can solve the series of equations and determine quantities of interest (QoI). A traditional solver accepts a set of inputs and produces a set of single-valued outputs. For instance, a solver might solve equations related to the attenuation of a beam of photons through a material, and the QoI might be the strength of the beam exiting the material. A single run of the solver usually results in a single value, or realization, of the quantity of interest.

This single realization might be misleading, however. In most systems there is some degree of uncertainty in the input parameters to the solver. Some of these uncertainties may be epistemic, or systematic uncertainty originating with inexact measurements or measurable unknowns. Other uncertainties might be aleatoric, intrinsic uncertainty in the system itself, such as probabilistic interactions or random motion. Taken together, the input parameter uncertainties exist within a multidimensional probabilistic space. While some points in that space may be more likely than others, the possible range of values for the QoI is only understood when the uncertain input space is considered as a whole. We note here that while it is possible that some of the input parameters are correlated in their probabilistic distribution, it is also possible to decouple them into uncorrelated variables. Throughout this work we will assume the input parameters are uncorrelated.

One traditional method for exploring the uncertain input space is through random sampling, such as in analog Monte Carlo sampling. In this method, a point in the input space is chosen at random based on probability. This point represents values for the input parameters to the solver. The solver is executed with these inputs, and the QoIs

are collected. Then, another point in the input space is chosen at random. This process continues until the properties of the QoIs, or *response*, are well understood.

There are some beneficial properties to random sampling approaches like Monte Carlo. Significantly, they are unintrusive: there is no need to modify the solver in order to use these methods. This allows a framework of algorithms to be developed which know only the input space and QoI of a solver, but need no further knowledge about its operation. Unintrusive methods are desirable because the uncertainty quantification algorithms can be developed and maintained separately from the solver.

Monte Carlo and similar sampling strategies are relatively slow to converge on the response surface. For example, with Monte Carlo sampling, in order to reduce the standard error of the mean of the response by a factor of two, it is necessary to take at least four times as many samples. If a solver is sufficiently computationally inexpensive, running additional solutions is not a large concern; however, for lengthy and expensive solvers, it may not be practical to obtain sufficient realizations to obtain a clear response.

In this work, we will assume solvers are computationally expensive, requiring many hours per solve, and that computational resource availability requires as few solves as possible. As such, we consider several methodologies for quantifying the uncertainty in expensive solver calculations. In order to demonstrate clearly the function of these methods, we apply them first on several simpler problems, such as polynomial evaluations and analytic attenuation. These models have a high degree of regularity, and their analyticity provides for straightforward benchmarking. Through gradual increasing complexity, we investigate the behavior of the UQ methods.

Finally, we apply the methods to an engineering-scale solver that models the neutronics of nuclear fuel. This will demonstrate the "real life" application of the uncertainty quantification methods, where the regularity and other properties of the model are not well understood.

The first uncertainty quantification method we consider is traditional analog Monte Carlo (MC) analysis, wherein random sampling of the input space generates a view of the response. MC is used as a benchmark methodology; if other methods converge on moments of the quantities of interest more quickly and consistently than MC, we consider them "better" for our purposes.

The second method we consider is stochastic collocation for generalized polynomial chaos (SCgPC)[11, 22–24], whereby deterministic collocation points are used to develop a polynomial-interpolated reduced-order model of the response as a function of the inputs. This method algorithmically expands the solver as the sum of orthogonal multi-dimensional polynomials with scalar coefficients. The scalar coefficients are obtained by

numerical integration using multidimensional collocation (quadrature) points. The chief distinction between SCgPC and Monte Carlo methods is that SCgPC is deterministic, in that the realizations required from the solver are predetermined instead of randomly sampled. There are two major classes of deterministic uncertainty quantification methods: intrusive and unintrusive. Like Monte Carlo, SCgPC is unintrusive and performs well without any need to access the operation of the solver. This behavior is desirable for construction black-box approach algorithms for uncertainty quantification. Other intrusive methods such as stochastic Galerkin exist [5], but require solver modification to operate. This makes them solver-dependent and undesirable for an independent uncertainty quantification framework.

The other methods we present here expand on SCgPC. First, we introduce non-tensor-product methods for determining the set of polynomial bases to use in the expansion. Because a tensor product grows exponentially with increasing cardinality of the input space, we combat this curse of dimensionality using the alternative polynomial set construction methods[13]. These bases will then be used to construct Smolyak-like sparse grids [14] to provide collocation points that in turn calculate the coefficients in the polynomial expansion. Second, we consider anisotropic sparse grids, allowing higher-order polynomials for particular input parameters. We also consider methods for obtaining weights that determine the level of anisotropic preference to give parameters, and explore the effects of a variety of anisotropic choices.

The second method group we consider is high-dimension model representation (HDMR), which correlates with Sobol decomposition [20]. This method is useful both for developing sensitivities of the quantity of interest to subsets of the input space, as well as constructing a reduced-order model itself. We demonstrate the strength of HDMR as a method to inform anisotropic sensitivity weights for SCgPC.

Finally, we consider adaptive algorithms to construct both SCgPC and HDMR expansions using second-moment convergence criteria. We analyze these for potential efficiencies and shortcomings. We also propose future work to further improve the adaptive methods.

We implement all these methods in Idaho National Laboratory's `raven`[9] uncertainty quantification framework. `raven` is a Python-written framework that non-intrusively provides tools for analysts to quantify the uncertainty in their simulations with minimal development. To demonstrate the application of the method developed, we use a complex non-linear multiphysics system solver simulating the operation of a fuel pin within a nuclear reactor core, including both neutronics and fuel performance physics kernals. For this solver, we use the coupled `rattleSNake`[10] and `bison` [6, 8] production codes. Both of these codes are developed and maintained within the `moose`[7] environment. The

multiphysics nonlinear system provides a challenge with unknown response properties for the uncertainty quantification methods discussed in this proposal.

The remainder of this work will proceed as follows:

- Chapter 2: We mathematically describe the analytic problems solved by the simulations we will be running, along with their properties and inferences about the algorithms developed. We discuss potential approaches to model solving and applications of the models.
- Chapter 3: We describe methods for uncertainty quantification, including Monte Carlo and generalized Polynomial Chaos.
- Chapter 4: We analyze results obtained for SCgPC methods, and contrast them with traditional Monte Carlo convergence on statistical moments.
- Chapter 5: We describe implementation of HDMR, and adaptive methods for both SCgPC and HDMR. We discuss the strengths, weaknesses, and options for these adaptive methods.
- Chapter 6: We evaluate results for the adaptive methods in comparison with static methods and Monte Carlo. We again consider the strengths and weaknesses of the adaptive methods.
- Chapter 7: We draw conclusions from the evaluations performed, and offer some suggestions for applicability as well as future development.

Bibliography

[1] Ayres and Eaton. Uncertainty quantification in nuclear criticality modelling using a high dimensional model representation. *Annals of Nuclear Energy*, 80:379–402, May 2015.

[2] Rabiti, Cogliati, Pastore, Gardner, and Alfonsi. Fuel reliability analysis using bison and raven. In *PSA 2015 Probabilistic Safety Assessment and Analysis*, Sun Valley, Idaho, April 2015.

[3] McKay, Beckman, and Conover. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code, 1979.

[4] Wiener. The homogeneous chaos. *American Journal of Mathematics*, 60:897–936, 1938.

[5] Babuska, Tempone, and Zouraris. Galerkin finite element approximations of stochastic elliptic partial differential equations. *SIAM Journal on Numerical Analysis*, 42(2):800–825, 2004.

[6] Gleicher, Williamson, Ortensi, Wang, Spencer, Novascone, Hales, and Martineau. The coupling of the neutron transport application rattlesnake to the nuclear fuels performance application bison under the moose framework. Technical report, Idaho National Laboratory (INL), 2015.

[7] Gaston, Newman, Hansen, and Lebrun-Grandié. Moose: a parallel computational framework for coupled systems of nonlinear equations. *Nuclear Engineering and Design*, 239(10):1768 – 1778, 2009.

[8] Newman, Hansen, and Gaston. Three dimensional coupled simulation of thermomechanics, heat, and oxygen diffusion in nuclear fuel rods. *Journal of Nuclear Materials*, 392(1):6 – 15, 2009.

[9] Rabiti, Alfonsi, Mandelli, Cogliati, and Kinoshita. Raven, a new software for dynamic risk analysis. In *PSAM 12 Probabilistic Safety Assessment and Management*, Honolulu, Hawaii, June 2014.

[10] Wang. Nonlinear diffusion acceleration for the multigroup transport equation discretized with sn and continuous fem with rattlesnake. In *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013)*, Sun Valley, Idaho, May 2013.

[11] Xiu and Karniadakis. The wiener–askey polynomial chaos for stochastic differential equations. *SIAM Journal on Scientific Computing*, 24(2):619–644, 2002.

[12] Askey and Wilson. Some basic hypergeometric orthogonal polynomials that generalize jacobi polynomials. *Memoirs of the American Mathematical Society*, 54:1–55, 1985.

[13] Novak and Ritter. The curse of dimension and a universal method for numerical integration. In Günther Nürnberger, JochenW. Schmidt, and Guido Walz, editors, *Multivariate approximation and splines*, volume 125 of *ISNM International Series of Numerical Mathematics*, pages 177–187. Birkhäuser Basel, 1997.

[14] Smolyak. Quadrature and interpolation formulas for tensor products of certain classes of functions. In *Dokl. Akad. Nauk SSSR*, volume 4, page 123, 1963.

[15] Trefethen. Is guass quadrature better than clenshaw-curtis? *SIAM Review*, 50(1): 67–87, 2008.

[16] Gerstner and Griebel. Dimension-adaptive tensor-product quadrature. *Computing*, 71, 2003.

[17] Boulore, Struzik, and Gaudier. Uncertainty and sensitivity analysis of the nuclear fuel thermal behavior. *Nuclear Engineering and Design*, 253:200–210, 2012.

[18] Argonne National Laboratory. Argonne code center: benchmark problem book. *ANL-7416 M&C Division of ANS*, 1968.

[19] Babuska, Nobile, and Tempone. A stochastic collocation method for elliptic partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 45, 2007.

[20] Li, Rosenthal, and Rabitz. High dimensional model representations. *J. Phys. Chem. A*, 105, 2001.

[21] Hu, Smith, Willert, and Kelley. High dimensional model representations for the neutron transport equation. *NS&E*, 177, 2014.

[22] Nobile, Tempone, and Webster. A sparse grid stochastic collocation method for partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 46, 2008.

[23] Barthelmann, Novak, and Ritter. High dimensional polynomial interpolation on sparse grids. *Advances in Computational Mathematics*, 12, 2000.

[24] Bungartz and Griebel. Sparse grids. *Acta Numerica*, 13, 2004.

[25] Le Maître and Knio. *Spectral methods for uncertainty quantification with applications to computational fluid dynamics*. Springer, 1st edition, 2010.

[26] Fichtl and Prinja. The stochastic collocation method for radiation transport in random media. *J. Quantitative Spectroscopy & Radiative Transfer*, 12, 2011.

[27] Rising, Prinja, and Talou. Prompt fission neutron spectrum uncertainty propagation using polynomial chaos expansion. *Nucl. Sci. Eng.*, 175, 2013.