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Doctoral Thesis

Advanced Methods in Stochastic Collocation for Polynomial Chaos in RAVEN

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Abstract

As the complexity of experiments in fields such as nuclear engineering continues to increase, so too does the demand for robust computational methods to simulate these experiments in virtual space. In many of these simulations, exact input design parameters as well as intrinsic properties of the experiment are often sources of input uncertainty. Often, small perturbations in these uncertain parameters have significant impact on the outcome of an experiment. For instance, when considering nuclear fuel performance experiments, small changes in the thermal conductivity of the fuel can greatly affect the maximum stress on the surrounding cladding. In recent years quantifying the impact of the input uncertainties in such an experimental system has grown as the complexities in these systems increase. For some problems, the input parametric space and corresponding quantity of interest output space is sufficiently explored with a few low-cost computational calculations. For others, however, the computational model is costly and it takes a great many random samples to obtain a good understanding of the output space. 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 isotropic tensor product (TP) SCgPC, then expand to consider truncated polynomial spaces using total degree (TD) and hyperbolic cross (HC) construction strategies. Next, we consider applying anisotropy to the polynomial space construction, and analyze methods whereby the level of anisotropy can be approximated. This leads to introducing the Sobol decomposition method, or high-dimensional model representation (HDMR) method, both as a reduced-order model and as a method of obtaining sensitivity indices for informing anisotropic SCgPC. We analyze these methods on nontrivial neutron diffusion transport problems. Finally, we propose implementing adaptive algorithms for building both the polynomial space for SCgPC and the constituent subset space of HDMR in order to approach ideal efficiency in modeling high-dimension problems. Further, we propose implementing these methods in the uncertainty qunatification framework RAVEN and applying them to nuclear fuels performance code BISON.

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Chapter 1

Introduction

Fuels performance codes are numerical simulations intended to characterize the performance of a set of materials in a particular geometry under a certain environment, over time. The environmental considerations might include temperature, neutron flux, external pressure, and similar factors. In many cases, the performance is quantified by considering the maximum stress undergone by cladding around the fuel as it expands and makes contact. By varying the construction materials and geometry of the fuel, its cladding, and the gap between them, fuel can be designed for optimal performance without experiencing a rupture or similar break.

There are a plethora of parameters that go into simulating fuel performance. The fuel itself is made up of many constituent materials with a variety of densities and structures, as well as behavior under irradiation. The contents of the fuel-cladding gap determine how effectively heat can conduct out of the fuel and to the cladding, then out to a moderator, and the thickness of this gap determines the amount of fuel expansion allowed before contact is made and outward pressure begins increasing. The material and geometry of the cladding determine limits on stress and efficiency of heat transfer. Any of the material properties in the fuel, gap, or cladding, along with the environmental conditions, can be a source of uncertainty in determining the maximum stress applied to the cladding.

There are two categories into which sources of uncertainty fall: aleatoric, or the statistical uncertainty inherent in a system; and epistemic, or the systematic uncertainty due to imprecision in measurement or existence of measurable unknowns. While there are aleatoric uncertainties in fuel performance (such as the neutronics of irradiated fuel), in this work we consider mostly epistemic uncertainties surrounding the material properties and geometries of the problems. For an example case, we can consider the overall reactor power, fuel mesoscale grain growth, and fuel thermal expansion coefficient as uncertain

input parameters, with maximum Von Mises stress in the axial center of a fuel rod as a quantity of interest in the output space.

In this work, we consider several methodologies for quantifying the uncertainty in fuel performance calculations. In order to demonstrate clearly the function of these methods, we demonstrate them first on several simpler problems, such as polynomial evaluations or projectile motion. The first method we consider is traditional, analog Monte Carlo (MC) analysis, wherein random sampling of the input space generates a view of the output space. MC is used as a benchmark methodology; if other methods converge on quantities of interest more quickly and accurately than MC, we consider them "better" for our purposes.

The second method we consider is isotropic, tensor-product (TP) stochastic collocation for generalized polynomial chaos (SCgPC)[1][2][3][4], whereby deterministic collocation points are used to develop a polynomial reduced-order model of the output quantities of interest as a function of the inputs. The other methods we consider expand on this method. First, we introduce non-tensor-product methods for determining polynomial bases, using the total degree (TD) and hyperbolic cross (HC) polynomial set construction methods[5]. These bases will then be used to construct Smolyak-like sparse grids for collocation[6]. Second, we consider anisotropic sparse grids, allowing additional collocation points for preferential input parameters. We also consider methods for determining weights that determine the level of preference to give parameters, and explore the effects of a variety of anisotropic choices.

The third method we consider is high-dimension model representation (HDMR), which correlates with Sobol decomposition [7]. 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.

Additionally, we propose continued work on developing adaptive algorithms for both SCgPC and HDMR[8]. In adaptive SCgPC, the polynomial basis is constructed level-by-level based on the highest-impact subset polynomials. In adaptive HDMR, the constituent subset input spaces are developed similarly, based on the highest-impact input subset. The crowning achievement we propose is combining HDMR and SCgPC to develop both the subset input space as well as the overall reduced-order model adaptively in an attempt to construct a competitively-efficient method for uncertainty quantification.

Finally, we propose all these methods be developed within 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 impact. `RAVEN` has already been shown to work seamlessly with `MOOSE`-based fuel performance code `BISON`[10][11], on which we propose to demonstrate the various methods described above.

The remainder of this work will proceed as follows:

- Chapter 2: We mathematically describe the problems solved by the simulations we will be running, including polynomial evaluations, attenuation, projectile, diffusion, and fuel performance. We discuss their potential applications and approach using random sampling.
- Chapter 3: We describe our implementation of SCgPC, including isotropic and anisotropic, as well as TP, TD, and HC construction strategies.
- Chapter 4: We describe our implementation of HDMR, and its possible applications as both a reduced-order model and a method for determining sensitivity coefficients.
- Chapter 5: We discuss proposed work extending both SCgPC and HDMR to be constructed adaptively. We also discuss the predicted shortfalls in the adaptive algorithms and some potential methods to address them.

Chapter 2

Simulation Physics

2.1 Simulations Used

To demonstrate the efficacy of the various uncertainty quantification methods we use in this work, we employ several independent simulations (hereafter referred to as "codes") of increasing complexity. These codes range from simple polynomial evaluations to analytic solutions of simple physics, to nonlinear multistage iterative solvers representing complex codes. We describe each briefly here.

2.2 Polynomial Evaluations

In order to benchmark the simplest cases, we make use of simple polynomial expressions of the form

$$u(Y) = \prod_{i=1}^{N} (y_i^b + a), \tag{2.1}$$

where $u(Y)$ is the quantity of interest, $Y = [y_1, y_2, \ldots, y_N]$ is the vector of uncertain inputs, and a and b are arbitrary scalar values. The input variables Y can be distributed arbitrarily. These polynomials are demonstrations where SCgPC evaluates exactly at some finite expansion level.

2.3 Attenuation

To demonstrate the convergence rates of various methods, we make use of an adjusted attenuation problem that is equivalent to the penetration of point particles in a purely-absorbing medium. The uncertain input variables are each the length of a segment of

material, and each segment has an identical cross section equal to 1. The quantity of interest is the percentage of particles exiting the material. We normalize the length of the segments to preserve significant values for the percentage exiting. The solution to this problem is

$$u(Y) = \prod_{i=1}^{N} e^{-Y_i/L}, \tag{2.2}$$

$$u(Y) = \sum_{i=1}^{N} \exp\left[\frac{\sum_{i=1}^{N} -Y_i}{L}\right], \tag{2.3}$$

where $L = |Y|_1$ is the total segment length. The input variables Y can be distributed arbitrarily.

The benefit of this model is a simple analytic solution, which makes analytic benchmarks possible. In addition, because of the exponential form, SCgPC will converge on a solution, but not replicate it exactly as in the polynomial case. This allows accurate comparison between MC, SCgPC methods, and HDMR methods.

2.4 Projectile

For a nonlinear case without an analytic solution, we consider the path traveled by a projectile near the surface of the Earth, considering varying gravitational pull with height as well as drag on the projectile from stagnant air. The equations governing travel in both vertical position x and horizontal position y are given by

$$y(t) = \frac{v_T}{g}(v\sin\theta + v_T)\left(1 - \exp\left[\frac{-gt}{v_T}\right]\right) - v_T t, \tag{2.4}$$

$$x(t) = \frac{v v_T \cos\theta}{g}\left(1 - \exp\left[\frac{-gt}{v_T}\right]\right), \tag{2.5}$$

where t is time, g is acceleration due to gravity, v is scalar velocity, θ the angle between the velocity vector and the horizontal ground, $v_T = \frac{mg}{D}$ is terminal velocity, $D = \frac{\rho C A}{2}$ is the acceleration due to drag, C is the drag coefficient, and $A = \pi r^2$ is the surface area of the projectile in the direction of travel. The projectile is assumed to present an identical surface area in both x and y directions. The quantity of interest is the range, or the total distance in x traveled by the ball before reaching a height of $y = 0$. The uncertain input variables are distributed uniformly as described in Table 2.1.

This simulation has the benefit of an analytic solution when $C = 0$ and eight distinct input parameters of varying importance. This is especially useful in considering anisotropic treatment of the input space.

Variable	Name	Mean	Range (±)	Units
y_i	Initial Height	1	1	m
v	Initial Velocity	35.5	2.5	m/s
θ	Initial Angle	45	10	degrees
g	Accel. Gravity	9.79888	0.0349	m/s/s
m	Projectile Mass	0.145	0.0725	kg
r	Projectile Radius	0.0336	0.00336	m
C	Drag Coefficient	0.5	0.5	
ρ	Air Density	1.2	0.1	kg/m^3

TABLE 2.1: Projectile Problem Distributions

2.5 Neutron Diffusion

For a nonlinear system with complicated physics, we consider a two-group, two-dimensional neutron diffusion criticality calculation. We make use of the diffusion approximation for neutron transport, which provides us with a coupled set of elliptic PDEs to solve:

$$-\boldsymbol{\nabla}\cdot(D_1(\bar{x})\boldsymbol{\nabla}\phi_1(\bar{x}))+\Big(\Sigma_a^{(1)}(\bar{x})+\Sigma_s^{(1\to 2)}(\bar{x})\Big)\phi_1(\bar{x})=\frac{1}{k(\phi)}\sum_{g'=1}^{2}\nu_{g'}\Sigma_f^{(g')}(\bar{x})\phi_{g'}(\bar{x}), \quad (2.6)$$

$$-\boldsymbol{\nabla}\cdot(D_2(\bar{x})\boldsymbol{\nabla}\phi_2(\bar{x}))+\Sigma_a^{(2)}(\bar{x})\phi_2(\bar{x})=\Sigma_s^{(1\to 2)}(\bar{x})\phi_1(\bar{x}), \quad (2.7)$$

where we use the following parametric coefficients: the absorption cross section $\Sigma_{g,a} = \Sigma_{g,c} + \Sigma_{g,f}$; the capture and fission cross sections $\Sigma_{g,c}$ and $\Sigma_{g,f}$; the diffusion coefficient D_g which depends on the scattering cross section of the medium; and the fission multiplication factor ν_g, the ratio of new neutrons per fission-producing neutron. The solution to this PDE is the neutron scalar flux $\phi_g(\bar{x})$. We apply no-traction conditions on the vacuum boundaries and zero-derivative current on the reflecting boundaries for both energy groups:

$$\frac{\phi_g}{4}-\frac{D_g}{2}\left.\frac{\partial\phi_g}{\partial x_1}\right|_{\partial\Omega_{\text{top}}}=0,\ \ g=1,2, \quad (2.8)$$

$$\frac{\phi_g}{4}-\frac{D_g}{2}\left.\frac{\partial\phi_g}{\partial x_2}\right|_{\partial\Omega_{\text{right}}}=0,\ \ g=1,2, \quad (2.9)$$

$$-D_g\left.\frac{\partial\phi_g}{\partial x_1}\right|_{\partial\Omega_{\text{bottom}}}=0,\ \ g=1,2, \quad (2.10)$$

$$-D_g\left.\frac{\partial\phi_g}{\partial x_2}\right|_{\partial\Omega_{\text{left}}}=0,\ \ g=1,2. \quad (2.11)$$

The criticality eigenvalue and quantity of interest $k(\phi)$ is given by

$$k(\phi) = \sum_{g=1}^{2} \iint_{D} \frac{\nu\Sigma_f^{(g)}\phi_g(\bar{x})}{\left(-\nabla \cdot D_g \nabla + \Sigma_r^{(g)}\right)\phi_g(\bar{x})}\, d\bar{x}. \tag{2.12}$$

We address solving ϕ_1, ϕ_2, and k nonlinearly and simultaneously. The material properties are shown in Table 2.2, and the domain $\Omega = [0, 200 \text{ cm}]^2$. The reference flux solutions are plotted in Fig. 2.2, and for the reference problem k=1.00007605445.

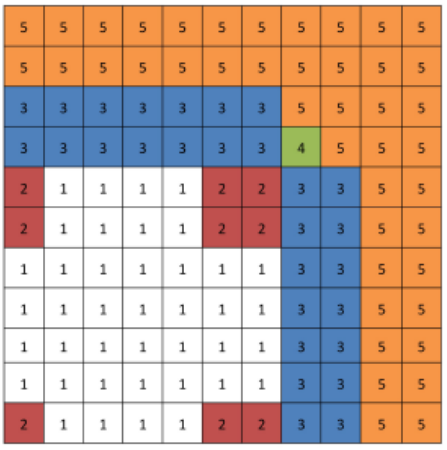
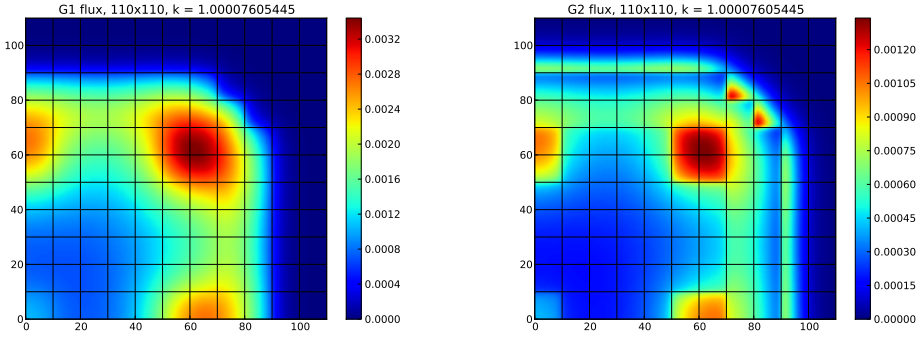


FIGURE 2.1: Core Geometry

Region	Group	D_g	$\Sigma_{a,g}$	$\nu\Sigma_{f,g}$	$\Sigma_s^{1,2}$
1	1	1.255	8.252e-3	4.602e-3	2.533e-2
	2	2.11e-1	1.003e-1	1.091e-1	
2	1	1.268	7.181e-3	4.609e-3	2.767e-2
	2	1.902e-1	7.047e-2	8.675e-2	
3	1	1.259	8.002e-3	4.663e-3	2.617e-2
	2	2.091e-1	8.344e-2	1.021e-1	
4	1	1.259	8.002e-3	4.663e-3	2.617e-2
	2	2.091e-1	7.3324e-2	1.021e-1	
5	1	1.257	6.034e-4	0	4.754e-2
	2	1.592e-1	1.911e-2	0	

TABLE 2.2: Reference Material Properties for Benchmark Core



(A) ϕ, Group 1 (B) ϕ, Group 2

FIGURE 2.2: Reference Flux Profiles

2.6 Fuel Rod Performance

While the previous codes were designed and written by the author, `BISON` is a professional use code maintained by Idaho National Laboratory. The fuel performance simulation used in this work is described in [12], and involves an axial-symmetric LWR fuel rodlet, composed of ten uranium dioxide pellets, zirconium-4 cladding, gap, and upper plenum. The problem is a power ramp-up transient as delineated in Table 2.3. The three uncertain input parameters are distributed in a truncated normal and are shown in Table 2.4. Note that scaling parameters are used for both grain radius and reactor power, such that a scaling factor of one is the nominal unperturbed case.

Time (s)	Linear Power (W/m)
0	0
1e4	3.5e4
1.5e8	3.5e4

TABLE 2.3: Linear Power Time Evolution

Variable	Min. Value	Max. Value
Grain Radius Scale Factor	0.4	1.5
Thermal Expansion Coefficient	9e-6	1.1e-5
Linear Power Scaling Factor	0.95	1.05

TABLE 2.4: Fuel Performance Input Distributions

The quantity of interest are the stresses on the axial center of the cladding. The uncertain parameters used in this test case are the mesoscale grain radius of the fuel, the simulated power of the reactor surrounding the fuel rod, and the thermal expansion coefficient of the fuel.

Chapter 3

Stochastic Collocation and generalized Polynomial Chaos

3.1 Uncertainty Quantification Methods

We consider a few methods for uncertainty quantification (UQ). One method to classify UQ methods is by their interaction level with a simulation code. Non-intrusive methods treat the code as a black box, perturbing the inputs and collecting the outputs without modifying the code. These methods are ideal for generic application frameworks, where the simulation code may be unknown or precompiled. Examples of non-intrusive methods include analog Monte Carlo (MC), Latin Hypercube sampling (LHS), and deterministic collocation methods. Alternatively, intrusive methods require access to the solution algorithm itself. Sometimes this can provide more efficient solutions. In particular, adjoint methods require the solution operator to be reversible, and provide very efficient methods to determine sensitivities and analyze output-input dependence. While many intrusive methods have benefits, they lack the flexibility and universal applicability of non-intrusive methods, and so we neglect them in this work.

3.2 Correlation

An assumption we make going forward is that the uncertain input parameters are independent or at least uncorrelated. If this is not the case, methods such as Karhunen-Loeve expansion can be used to develop an orthogonal input space to replace the original. Similarly, principle component analysis can be used to attempt to find the fundamental uncorrelated space that maps into the correlated variable space.

3.3 Monte Carlo

In analog Monte Carlo uncertainty quantification, a single point in the input space is selected randomly, and an output collected, until an appropriately accurate view of the output space is acquired. While few samples result in a poor understanding of the quantity of interest, sufficiently large samples converge on a correct solution. The convergence rate of Monte Carlo is consistent, as

$$\epsilon = \frac{c}{\sqrt{\eta}}, \tag{3.1}$$

where c is a constant and η is the number of samples taken. While this convergence rate is slow, it is possibly one of the most reliable methods available. This makes MC a good choice for benchmarking.

One of the downsides of MC (and LHS) when compared with other methods is that they do not generate a reduced-order model as part of the evaluation; however, interpolation methods can be used to generate additional samples.

3.4 Latin Hypercube Sampling

Latin hypercube sampling[13] is another stochastic method that specializes in multidimensional distributions.

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