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Adjoint-Based Uncertainty Quantification for Radiation Transport Calculations with Uncertain Cross-Section Data

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Abstract - *An original approach to uncertainty quantification (UQ) for radiation transport problems with uncertain nuclear data is introduced in this paper. A novel dimension-reduction scheme is applied to the nuclear data characterizing cross-section uncertainty. An adjoint-based sensitivity analysis is performed to yield sensitivity coefficients for a quantity of interest (QoI) with respect to the multigroup cross sections and then mapped to the reduced-dimensional space. Finally, response surfaces or emulators are constructed for the QoI over the reduced-dimensional space. These surfaces yield information about the distribution of the QoI in the original uncertain input space. This multi-step approach is applied to a radiation transport problem for which traditional UQ methods are prohibitively expensive.*

I. INTRODUCTION

The accurate modeling of complex phenomena such as radiation transport in a laboratory experiment challenges the limits of modern computing resources and motivate the design of next-generation exascale computers. The efficient and accurate propagation of uncertainty through these problems is an area of ongoing research. Understanding and quantifying uncertainty in quantities of interest (QoIs) that arise due to uncertain material properties is a vital component of predictive calculations. A response surface or emulator is one tool that can be used to investigate the contribution of uncertainty in input parameters to uncertainty in a QoI, but the cost of constructing an accurate surrogate model grows exponentially as the dimensionality of the uncertain input space increases.

Nuclear cross sections are one source of uncertainty in neutron transport calculations. These cross sections define the interaction probability of neutrons in a material. A deterministic neutron transport problem may require thousands of cross sections as input. Although tools exist to characterize and quantify the uncertainty in these cross sections, the dimensionality of this uncertain parameter space poses a significant challenge for traditional methods of UQ analysis.

A novel dimension-reduction scheme for cross section uncertainty is outlined in this work and applied to the modeling of a laboratory experiment. This scheme combines a decomposition of the uncertain cross sections' covariance matrix, forward and adjoint-sensitivity transport calculations performed at various points in the uncertain-parameter space, and a first-order sensitivity analysis. A decomposition of the covariance matrix characterizing the uncertainty in the cross section data yields a set of independent, unit-normal uncertain parameters and establishes a mapping between this independent-parameter space and the cross-section space. Samples of the uncertain cross-section space are obtained by sampling the independent-parameter space and mapping the samples to the cross-section space. A pair of forward and adjoint calculations are performed at each realization of the cross sections to calculate the partial derivative of the QoI with respect to each cross section. These cross-section sensitivity coefficients are mapped to the independent parameters, yielding partial derivatives of the QoI with respect to the independent parameters. Finally, a first-order sensitivity analysis is used to estimate the relative contribution of each independent parameter to the uncertainty in the QoI. Important independent parameters are identified based on these relative contributions to the total uncertainty in the QoI.

The greatly reduced dimensionality of the important parameter space makes the construction of a surrogate model tractable. Given a response surface that accurately models the distribution of a QoI, the surface may be used as an emulator to supplement or supplant the full code for some analyses [1]. A Monte Carlo analysis may be performed by drawing hundreds of thousands or millions of samples from the emulator to determine the distribution of the QoI over the uncertain-parameter space. In order for a response surface to be useful for these purposes, it must be both accurate and predictive. The construction of a surface that satisfies both of these characteristics is outlined in the following pages.

In the following sections we will outline the generation of the data describing the uncertain cross sections, the derivation of the adjoint sensitivity method, the novel dimension reduction method, and the construction of a response surface in terms of these important parameters. Finally, results are presented for a complex problem related to a laboratory experiment being performed at Texas A&M University.

II. NUCLEAR DATA AND MULTIGROUP CROSS SECTION PREPARATION

The transport of neutrons through a laboratory experiment or nuclear reactor is described by the linear Boltzmann equation, commonly referred to as the radiation transport equation. The interaction of neutrons in a bulk material is characterized by the material's macroscopic cross section, which is the product of isotope-specific microscopic cross sections and the atom densities of the isotopes present in the bulk material. The microscopic cross sections are analyzed as the uncertain

parameters of interest in this work.

Cross-section data is generated by theoretical calculation and by direct experimentation, each of which give rise to uncertainties in the cross sections. The process of collecting data from various experiments and calculations and producing a cohesive nuclear data set is called evaluation. Evaluated nuclear data is collected in data sets called the Evaluated Nuclear Data Files (ENDF) [2]. These files contain both the best estimate of the energy-dependent cross sections and an estimate of the uncertainty in these cross sections. The ENDF contain both extremely fine pointwise data and resonance parameters that describe the resolved- and unresolved-resonance regions of the cross sections.

The continuous energy cross-section data is discretized in energy by the multigroup method. The multigroup method approximates the cross sections as a collection of piecewise constant step functions in energy. The code NJOY 2012 [3] was used to process the ENDF/B-VII.1 data to produce multigroup cross sections and their associated uncertainty.

NJOY 2012 processes the ENDF/B-VII.1 data and produces the zeroth and first moments of the multigroup cross sections. The zeroth moment $\vec{x}_\mu$ is the best estimate of the value of the cross sections. These will be referred to as the mean value of the cross sections. The first moment of the cross-section distribution describes the uncertainty in the cross-section values as well as the correlations that exist across energy and across different reactions. This is contained in a covariance matrix $\overline{\overline{\Sigma}}_x$. Given $\vec{x}_\mu$ and $\overline{\overline{\Sigma}}_x$, the multigroup cross sections $\vec{x}$ may be approximated as a multivariate Gaussian distribution,

$$\vec{x} \sim N(\vec{x}_\mu, \overline{\overline{\Sigma}}_x). \tag{1}$$

Drawing from this distribution generates realizations R_i of the cross sections $\vec{x}_{R_i}$ that reflect both the recorded uncertainty in the data and the correlations across energy groups and interactions.

NJOY produces covariance data for all reactions that result in the removal of a neutron from an energy group, including absorptive reactions such as (n,γ) and (n,α), and the total scattering probability from each group g, that is, the sum of the scattering cross sections from group g to all groups g'. Realizations of the group-to-group scattering cross sections are generated by assuming that the ratio of scattering from group g to each group g' is constant across all realizations of the cross sections.

For a given isotope, the multigroup cross sections are correlated across energy groups for a given reaction and may be correlated across nuclear reactions. Although covariances may be observed across isotopes (as in the related work [4]), these are only generated by NJOY in the case in which only the total, scattering, and fission cross sections are generated; at present, if specific absorptive reactions are desired, NJOY 2012 will not report cross-isotope covariances. For this reason cross-isotope terms were not considered in this work.

The mean value of the multigroup cross sections and realizations drawn from the multivariate Gaussian distribution defined by $\vec{x}_\mu$ and $\overline{\overline{\Sigma}}_x$ are formatted as nuclear data files to be read by the deterministic neutron transport code PDT (described in the following Section).

III. THE NEUTRON TRANSPORT EQUATION

The behavior of neutrons in a background material is accurately described by the linear Boltzmann equation for sparse gases, which is also known as the radiation transport equation [5]. The principal unknown is the neutron angular flux ψ, which has units of neutrons per second per steradian per energy per centimeter squared. The angular flux depends upon independent parameters in time t, space r, angle Ω, and energy E. The steady state form of this equation in non-multiplying media is

$$\vec{\Omega} \cdot \nabla\psi(\vec{r}, E, \vec{\Omega}) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \vec{\Omega}) = \int_{4\pi}\int_0^\infty \Sigma_s(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega})\psi(\vec{r}, E', \vec{\Omega}')dE'd\vec{\Omega}' + s(\vec{r}, E, \vec{\Omega}, t). \tag{2}$$

Here Σ_t and Σ_s are the macroscopic total and scattering cross sections, respectively, with units of 1/cm, and s is a source term with units of neutrons per cm^2 per second per steradian.

1. Discretization of the Neutron Transport Equation

This equation must be discretized in space, angle, and energy. The discretization schemes used in this work through the research code "PDT" under development at Texas A&M University are mentioned here. The angular flux variable is discretized in angle using the discrete ordinates (S_N) approximation with a product Gauss Legendre Chebyshev quadrature set [6][7], in energy using the multigroup approximation [3], and in space with the piece-wise linear discontinuous (PWLD) spatial discretization [8][9].

The discretization of the transport equation in space, angle, and energy yields a collection of coupled equations. For convenience these coupled equations are often written in operator or matrix form. In this notation the fully discretized angular flux is represented as the vector $\vec{\psi}$. The streaming and total interaction terms are collected into the matrix $\overline{\overline{L}}$, the anisotropic scattering operator is represented $\overline{\overline{S}}$, and the inhomogeneous neutron source is represented as $\vec{q}$. Combining these, and neglecting the matix and vector notation for compactness, the radiation transport equation can be succinctly written

$$L\psi = S\psi + q. \tag{3}$$

This compact notation for the fully discretized transport equation will be used from this point forward.

2. The Adjoint Sensitivity Method

The adjoint sensitivity method is an extremely efficient means by which sensitivity coefficients for a problem containing a large number of parameters of interest and a small number of quantities of interest may be calculated [10]. A brief overview of the derivation of the adjoint sensitivity equations for the radiation transport equations is presented here, following the work of [11], [12], and [13].

An inner product is required for this derivation. Let us define the inner product of vectors $\vec{a}$ and $\vec{b}$ as the integral over all phase space of these two vectors,

$$\langle a, b\rangle = \int_{4\pi} d\Omega \int_{\mathcal{D}} dV \int_0^\infty dE a(\vec{r}, \vec{\Omega}, E) b(\vec{r}, \vec{\Omega}, E). \quad (4)$$

As these inner products will be applied to the operator form of the transport equation, we neglect the vector notation for $\vec{a}$ and $\vec{b}$ within the angle brackets.

For vectors of the discretized angular flux, this integration is accomplished by summing the cell-averaged values a_{c_A} and b_{c_A} over the energy groups g, discrete angles d with associated quadrature weights w_d, and spatial cells c with volumes V_c. This summation is

$$\langle a, b\rangle = \sum_d w_d \sum_c V_c \sum_g a_{c_A,d,g} b_{c_A,d,g}. \quad (5)$$

The quantities of interest Q examined in this work are reaction rates, which are integral quantities of the scalar flux and the macroscopic cross section corresponding to the reaction of interest in a region of interest such as a detector volume, Σ_r. The QoI Q may be expressed as the inner product

$$Q = \langle \Sigma_r, \psi \rangle . \quad (6)$$

The derivation of the adjoint sensitivity equations begins by forming a Lagrangian system $\mathcal{L}$ by taking an inner product of the discretized radiation transport equation Eq (3) with an as-of-yet undefined adjoint function $\psi^\dagger$ and subtracting it from the QoI, Eq. (6),

$$\mathcal{L} = \left\langle \psi, q^\dagger \right\rangle - \left\langle \psi^\dagger, L\psi \right\rangle + \left\langle \psi^\dagger, S\psi \right\rangle + \left\langle \psi^\dagger, q \right\rangle . \quad (7)$$

We will see that the as-yet-undefined $\psi^\dagger$ is a Lagrangian multiplier. As long as ψ satisfies the forward problem, the Lagrangian is identically equal to the QoI. The derivative of $\mathcal{L}$ with respect to an uncertain parameter p is obtained through the chain rule,

$$\frac{d\mathcal{L}}{dp} = \frac{\partial \mathcal{L}}{\partial p} + \frac{\partial \mathcal{L}}{\partial \psi}\frac{\partial \psi}{\partial p} + \frac{\partial \mathcal{L}}{\partial \psi^\dagger}\frac{\partial \psi^\dagger}{\partial p}. \quad (8)$$

Applying the chain rule to Eq. (7) and carefully organizing terms eventually yields

$$\begin{aligned}\frac{d\mathcal{L}}{dp} =& \left[\left\langle \frac{\partial}{\partial p}\psi, -L^\dagger\psi^\dagger + S^\dagger\psi^\dagger + q^\dagger \right\rangle \right. \quad (9)\\ &+ \left\langle \frac{\partial}{\partial p}\psi^\dagger, -L\psi + S\psi + q \right\rangle \\ &\left. + \left\langle \psi, \frac{\partial}{\partial p} q^\dagger \right\rangle - \left\langle \psi^\dagger, \left(\frac{\partial}{\partial p} L\right)\psi \right\rangle + \left\langle \psi^\dagger, \left(\frac{\partial}{\partial p} S\right)\psi \right\rangle \right] \\ &+ \left[\left\langle -L^\dagger\psi^\dagger + S^\dagger\psi^\dagger + q^\dagger \right\rangle\right] \frac{\partial \psi}{\partial p} \\ &+ \left[\langle -L\psi + S\psi + q\rangle\right] \frac{\partial \psi^\dagger}{\partial p}\end{aligned}$$

The difficult- or impossible-to-calculate terms $\frac{\partial \psi}{\partial p}$ and $\frac{\partial \psi^\dagger}{\partial p}$ are isolated as multipliers of the forward transport equation and the familiar adjoint radiation transport equation,

$$L^\dagger\psi^\dagger = S^\dagger\psi^\dagger + q^\dagger. \quad (10)$$

If the forward and adjoint transport equations are satisfied then the expression for the partial derivative of the QoI with respect to parameter p is

$$\frac{dQ}{dp} = \left\langle \psi, \frac{\partial}{\partial p} q^\dagger \right\rangle - \left\langle \psi^\dagger, \left(\frac{\partial}{\partial p} L\right)\psi \right\rangle + \left\langle \psi^\dagger, \left(\frac{\partial}{\partial p} S\right)\psi \right\rangle . \quad (11)$$

From this expression it is clear that for each QoI, two solutions of the radiation transport problem (one forward and adjoint) will yield any number of sensitivity coefficients at the cost of several inner products per parameter of interest. These inner product evaluations are inexpensive compared to the cost of solving the forward and adjoint radiation transport equations.

IV. A NOVEL DIMENSION REDUCTION SCHEME

The dimension-reduction scheme introduced in this section is notable for identifying a set of independent, unit-normal (Gaussian) parameters which preserve the correlations in the multigroup cross section data and give rise to the uncertainty in the QoI.

1. Identification of Independent, Unit-Normal Parameters

The multigroup cross sections produced from the ENDF/B-VII.1 data and NJOY 2012 are approximated as a multivariate Gaussian distribution with mean $\vec{x}_\mu$ and covariance matrix $\overline{\overline{\Sigma_x}}$. Let us denote the vector of multigroup cross sections $\vec{x}$ and use the subscript x to denote terms corresponding to the cross-section data,

$$\vec{x} \sim N(\vec{x}_\mu, \overline{\overline{\Sigma_x}}). \quad (12)$$

A computationally efficient method to sample a multivariate Gaussian distribution is presented in [14] and outlined here. To sample the cross-section distribution we must compute a matrix $\overline{\overline{A_x}}$ such that

$$\overline{\overline{A_x}}\,\overline{\overline{A_x}}^T = \overline{\overline{\Sigma_x}}. \quad (13)$$

A Cholesky factorization is often used to construct $\overline{\overline{A_x}}$. However, the covariance matrices generated from the evaluated nuclear data files with NJOY are not always symmetric positive definite, which can cause a Cholesky decomposition to fail. Instead let us take an eigenvalue decomposition of the covariance matrix

$$\overline{\overline{\Sigma_x}} = \overline{\overline{E_x}}\,\overline{\overline{\Lambda_x}}\,\overline{\overline{E_x^T}}. \quad (14)$$

The matrix $\overline{\overline{\Lambda_x}}$ is diagonal and contains the eigenvalues of $\overline{\overline{\Sigma_x}}$. The matrix $\overline{\overline{E_x}}$ contains the right eigenvectors corresponding

to the eigenvalues in $\overline{\overline{\Lambda}}_x$. Rewriting the matrix of eigenvalues $\overline{\overline{\Lambda}}_x$ as $\overline{\overline{\Lambda}}_x^{1/2}\overline{\overline{\Lambda}}_x^{1/2}$ shows that we can form a transform matrix $\overline{\overline{A}}_x$ that satisfies Eq. (13) as

$$\overline{\overline{A}}_x = \overline{\overline{E}}_x \overline{\overline{\Lambda}}_x^{1/2}. \tag{15}$$

Given the transform matrix $\overline{\overline{A}}_x$ calculated from the eigenvalue decomposition, we next define a vector $\vec{z}$ containing independent normal members z_i with mean zero and variance one,

$$z_i \sim N(0,1). \tag{16}$$

We refer to the $N(0,1)$ distribution as the "unit-normal" distribution and the parameters z_i as the "independent parameters." Denoting samples of the cross sections $\vec{x}$ and samples of the independent parameters $\vec{z}$ with a subscript R_i for "the i-th realization," samples of the cross-section space are produced as the product of $\overline{\overline{A}}_x$ and samples of $\vec{z}$,

$$\vec{x}_{R_i} = \overline{\overline{E}}_x \overline{\overline{\Lambda}}_x^{1/2} \vec{z}_{R_i} + \vec{x}_\mu. \tag{17}$$

The covariance matrix's eigenvalues may span tens of orders of magnitude. The entries in $\overline{\overline{\Lambda}}_x$ may be truncated after capturing the largest eigenvalue and all eigenvalues within several orders of magnitude of the dominant eigenvalue. In this work we retained the largest eigenvalue and all eigenvalues within eight orders of magnitude of the largest eigenvalue. The number of non-zero columns of the matrix $\overline{\overline{A}}_x$ (and therefore the number of meaningful entries in the vector $\vec{z}$) is equal to the number of retained eigenvalues in $\overline{\overline{\Lambda}}_x$. In practice, we have found that the number of non-zero rows of $\overline{\overline{A}}_x$ to be significantly smaller than the number of multigroup cross sections.

We note that the existence of these $\vec{z}$ parameters is not new to this work. Rather, these parameters are normally encapsulated within a third-party library used to sample multivariate Gaussian distributions. By performing this sampling ourselves these parameters are exposed for analysis. The significance of these $\vec{z}$ parameters is this: points in the multigroup cross section space may be uniquely defined as points in the smaller independent-parameter space and variations in the correlated multigroup cross-section space may be described by variations in these individual, independent, unit-normal parameters.

2. Mapping Between Cross Sections and Independent Parameters

A mapping can be defined for the transformation between the multigroup cross-section space and the independent parameter space by taking a derivative of Eq. (17) with respect to $\vec{z}$,

$$\frac{d\vec{x}}{d\vec{z}} = \frac{d}{d\vec{z}}\left(\overline{\overline{E}}_x \overline{\overline{\Lambda}}_x^{1/2}\vec{z} + \vec{x}_\mu\right), \tag{18}$$

yielding

$$\frac{\overline{\overline{dx}}}{dz} = \overline{\overline{E}}_x \overline{\overline{\Lambda}}_x^{1/2}. \tag{19}$$

A similar mapping can be defined for the derivatives of the QoI and the two spaces. The derivative of the QoI with respect to the parameters of interest is related to the derivative of the QoI with respect to the cross sections by the chain rule,

$$\frac{dQ}{dz} = \frac{dQ}{dx}\frac{dx}{dz}. \tag{20}$$

Accounting for the vector notation (and shapes) assumed thus far in the paper, this expression is

$$\frac{d\vec{Q}}{dz} = \frac{\overline{\overline{dx}}}{dz}^T \frac{d\vec{Q}}{dx}. \tag{21}$$

Substituting Eq (19) for the transform matrix $\frac{\overline{\overline{dx}}}{dz}$ and transposing the diagonal matrix of eigenvalues, this yields

$$\frac{d\vec{Q}}{dz} = \overline{\overline{\Lambda}}^{1/2} \overline{\overline{E_x}}^T \frac{d\vec{q}}{dx}. \tag{22}$$

Finally, for clarity let us replace the vectors of sensitivity coefficients $\frac{d\vec{Q}}{dx}$ and $\frac{d\vec{Q}}{dz}$ with $\vec{S}_x$ and $\vec{S}_z$, respectively,

$$\vec{S}_z = \overline{\overline{\Lambda}}_x^{1/2} \overline{\overline{E_x}}^T \vec{S}_x. \tag{23}$$

The sensitivity coefficients $\vec{S}_x$ are efficiently calculated using the adjoint sensitivity method outlined previously. This mapping from the partial derivatives of the QoI with respect to the multigroup cross sections to the partial derivatives of the QoI with respect to the independent parameters allows us to estimate the relative importance of each of these underlying parameters to the variance in the QoI.

3. Identification of Important Independent Parameters

The first-order sensitivity analysis (FOSA) method, or the "propagation of error" or "propagation of moments" equation, is commonly applied to estimate variance in a QoI σ_Q^2 due to some variables v given the covariance matrix $\overline{\overline{\Sigma}}_v$ and vector of sensitivity coefficients $\vec{S}_v$ [10],

$$\sigma_Q^2 = \vec{S}_v^{\,T} \overline{\overline{\Sigma}}_v \vec{S}_v. \tag{24}$$

From this equation we see that the uncertainty in a quantity of interest depends both on the sensitivity of that QoI to each uncertain variable S_v and the variances in and covariances between the variables v. Note that a variable with a large sensitivity does not necessarily give rise to a large variance in the QoI—if that variable is exactly known, it will not contribute any variance to the QoI. Alternatively, a variable with a large amount of uncertainty may contribute significant uncertainty to the QoI even if the sensitivity of the QoI to that variable is small.

The variance in the QoI can be estimated at each realization R_i of the cross section space by Eq. (24) using either the sensitivities and covariance matrix corresponding to the multigroup cross sections,

$$\sigma_Q^2\big|_{R_i} = \vec{S}_x\Big|_{R_i} \overline{\overline{\Sigma_x}}\ \vec{S}_x\Big|_{R_i}, \tag{25}$$

or the independent parameters,

$$\sigma_Q^2\Big|_{R_i} = \vec{S}_z\Big|_{R_i} \overline{\overline{\Sigma_z}}\ \vec{S}_z\Big|_{R_i}. \tag{26}$$

Because the z parameters are unit normal, the covariance matrix for the independent parameters $\overline{\overline{\Sigma_z}}$ is the identity matrix. Let us denote the number of z parameters as N_z. This means that Eq. (26) for the variance in the QoI reduces to the sum of the N_z squared sensitivity coefficients $\vec{S}_z$,

$$\sigma_Q^2\Big|_{R_i} = \sum_{j=1}^{N_Z} S_{z_j}^2\Big|_{R_i}. \tag{27}$$

An average variance in the QoI $\widehat{\sigma_Q^2}$ can be computed by averaging the local estimates of the variance computed at each of the M realizations of the cross section,

$$\widehat{\sigma_Q^2} = \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{N_Z} S_{z_j}^2\Big|_{R_i}. \tag{28}$$

The average contribution of the j-th independent parameter z_j to the variance in the QoI $\widehat{\sigma_Q^2}$ is denoted δ_j and is computed

$$\delta_j = \frac{1}{M}\sum_{i=1}^{M} S_{z_j}^2\Big|_{R_i}. \tag{29}$$

The fraction of the total variance contributed by each independent parameter z_j is easily calculated from Eq. (28) and Eq. (29). The independent parameters can be ordered from most important to least important by their contribution to the variance in the QoI δ_j. We denote the ordered average contributions to the average total variance by each z-parameter $\left[\delta_j\right]^{\text{ranked}}$ and indicate the index in this list with a subscript k. The K important independent parameters are chosen such that

$$\sum_{k=1}^{K} \frac{\left[\delta_j\right]_k^{\text{ranked}}}{\widehat{\sigma_Q^2}} \geq 1-\epsilon. \tag{30}$$

These K parameters are the important independent parameters that describe the variance in the QoI. In this work ϵ was set to 0.01, that is, parameters collectively responsible for approximately 99% of the variance were retained. This step tremendously reduces the number of dimensions that must be considered while retaining the dimensions responsible for almost all of the variance in the QoI.

In summary, the reduction of the multigroup cross-section space is accomplished in two distinct steps. First, an eigenvalue decomposition of the cross sections' covariance matrix is used to define a mapping between the cross-section space and a new, unit-normal independent-parameter space. This step is incidentally responsible for a decrease in the problem dimensionality. Second, sensitivity coefficients are mapped between the cross-section space and the independent-parameter space and and a first-order sensitivity analysis is performed at various points in the input space. From this FOSA, the relative contribution of each of the independent parameters to the variance in the QoI is estimated, allowing the identification of the important independent parameters. This importance-based ranking results in a very large reduction in the dimensionality of the problem of interest.

V. CONSTRUCTION AND USE OF A RESPONSE SURFACE WITH DAKOTA

A response surface or surrogate model is a mathematical model built to emulate the behavior of a complex computational model. These emulators are often constructed using evaluations of the full model at various points in the input space. These evaluations may include only the QoI at each point in the input space or may include local partial derivatives of the QoI with respect to the uncertain parameters. Many methods exist to construct a response surface from a collection of data, including Polynomial Chaos Expansions (PCEs), Gaussian Process Models (GPMs), kriging methods, Multivariate Adaptive Regression Splines (MARS) algorithms, and Bayesian MARS algorithms. In general, as the dimensionality of the input space increases, the difficulty of computing a response surface grows exponentially.

A response surface that accurately models the QoI as a function of the uncertain input parameters is useful for a variety of purposes [1]. As sampling the emulator is extremely efficient a Monte Carlo analysis may be performed using enough particles to thoroughly sample the uncertain parameter space. Local and global maxima and minima are easily identified for any range of the uncertain parameters.

The code package DAKOTA was used to construct a surrogate model given the QoI and sensitivity coefficients calculated at various points in the uncertain input space. A developmental branch of DAKOTA supports the construction of PCEs and GPMs using derivative information.[c] For this reason, these two models were utilized in this analysis. Further details on the implementation of these methods is available in the Dakota user's manual [15].

Even after reducing a problem's dimensionality by the identification of important parameters it may be computationally prohibitive or impossible to construct a response surface from only evaluations of the QoI at various points in the space. The availability of partial derivatives of the QoI with respect to each parameter at each sample of the input space may allow the construction of surrogate models for problems in which the dimensionality is otherwise prohibitive. The rate at which the PCE and GPM surrogates converge to an estimate for the mean and variance in the QoI with and without derivative information is examined in the following section.

VI. TEST PROBLEM AND RESULTS

The dimension reduction scheme introduced in this work was applied to a variety of test problems in [16]. A single problem modeling an ongoing laboratory experiment is presented in this section. The goal of the UQ analysis performed in this work is to calculate the quantity of interest and variance in the QoI for realistic neutron transport calculations using a gradient-informed response surface. The number of data points required to construct an accurate, predictive response surface is not known a priori. Therefore, for each test problem, the QoI's mean and variance are plotted versus the number of data points available to construct the surface.

The response surfaces are constructed in the independent-parameter space using an increasing pool of evaluations of

the forward and adjoint transport equations, starting with an evaluation at the mean value of the cross sections (which corresponds to all of the independent parameters being equal to zero). As the response surfaces are quick to generate compared to the cost of the forward and adjoint solves of the transport problem and the inner product evaluations, the surfaces could be constructed as QoI and sensitivity data is slowly generated.

The goal of this research is to produce accurate estimates of the mean and variance of a QoI for a complex problem with relatively few evaluations of the physics code at points in the input space. It is therefore desirable that the response surfaces converge rapidly as the number of data points is increased. Finally, it will prove interesting to compare the QoI and the variance in the QoI estimated by the first-order sensitivity analysis (FOSA) performed at the mean value of the cross sections to the results predicted by the response surfaces as the number of data points increase.

1. Problem Description

This research project was originally conceived to quantify the uncertainty in a predicted detector response due to uncertainty in the cross section data for an experiment being performed in the Nuclear Engineering Department at Texas A&M University. The Center for Exascale Radiation Transport (CERT) project, funded by the Predictive Science Academic Alliance Program II (PSAAP-II), seeks to predict the response of a detector placed in and around an complex graphite structure driven by a pulsed neutron source placed at one end of the structure. One series of experiments performed for this project, referred to here as the CERT experiment, involved the analysis of individual bricks of graphite.

The CERT experimental geometry involved an americium-beryllium (AmBe) neutron source located at the center and near the bottom of the large cylinder of high-density polyethylene (HDPE) on top of a wooden table. A graphite brick was placed on top of the HDPE cylinder. The HDPE thermalizes the neutrons before they enter the graphite brick. A BF_3 neutron detector was positioned above the graphite brick. Borated aluminum shielding was positioned around various components of the experiment.

The CERT experiment was modeled as a one-quarter geometry with reflecting boundary conditions. The spatial mesh contained on the order of 250,000 brick cells. A 49-group energy discretization was employed. The angular quadrature was specified with 12 polar and 6 azimuthal angles. The cross section data included a total of 14 isotopes and 17 nuclear reactions. The forward, adjoint, and inner product calculations required about six hours on 3,456 processors (216 nodes) on the supercomputer Vulcan, the open access version of Sequoia, at Lawrence Livermore National Laboratories to complete using this discretization scheme.

2. Test Results

The CERT problem was run at the mean value of the cross sections, $\vec{x}_\mu$ (alternatively expressed as $\vec{z} = 0$), and at one hundred samples of the input space drawn from uniform random distributions of the independent parameters. The independent parameters were sampled from uniform distributions in the range $[-3, 3]$; as each independent parameter is unit normal this corresponds to sampling a range about the mean of plus or minus three standard deviations.

Non-Zero Multigroup Cross Sections	3,287
Independent Parameters	1,344
Important Independent Parameters	4

TABLE I. Number of multigroup cross sections in the IM-1 problem, independent parameters revealed by the decomposition of the covariance matrix, and important independent parameters identified by the first-order sensitivity analysis.

The 101 IM-1 calculations collectively required about two million CPU hours on Vulcan to complete. The problem contained a total of 3,287 non-zero multigroup cross sections. The decomposition of the covariance matrices yielded 1,344 independent parameters. Finally, the dimension-reduction scheme identified four important independent parameters. These results are summarized in Table I.

Analysis of the transformation matrices used to map the independent z-parameters to the multigroup cross sections identified the cross sections which correspond to each important parameter. The most important parameter, responsible for more than 91% of the estimated total variance in the QoI, corresponded to elastic scattering and radiative capture in hydrogen in the HDPE. The remaining three important parameters were associated with the elastic, inelastic, and radiative capture cross sections of both hydrogen in the HDPE and carbon in the graphite. These results are summarized in Table II.

The QoI calculated at the 101 samples of the input space is plotted against the four important independent parameters in the top row of Figure (1). The partial derivative of the QoI with respect to the four important independent parameters is plotted in the bottom row of that figure. Note that the QoI appears to vary approximately linearly with respect to the first (and most important) independent parameter but does not seem to depend upon the other parameters. Also note that while the partial derivative of the QoI with respect to parameters P_2, P_3, and P_4 is very nearly constant across the range of those variables, the partial derivative of the QoI with respect to P_1 appears to vary linearly over the range of that variable.

Response surfaces were constructed with Dakota using data from the 101 adjoint sensitivity calculations performed on Vulcan. GPM and PCE surrogate models were constructed using increasing pools data from the calculations. Surrogates were constructed using only the QoI information (PCE and GPM models) and using both the QoI and derivative information; these "gradient-enhanced" models are referred to as the GE-PCE and GE-GPM models. The mean and standard deviation calculated with each of these surrogates are plotted in Figure 2 against the number of data points that were used in the construction of the surrogate model.

Both the GPM and PCE surrogate models converge to a QoI of approximately 4.35 counts / second in the detector volume and a standard deviation of approximately 0.09 counts / second, or approximately 2.1%. Both models demonstrated similar behavior as a function of the number of data points available to construct the response surfaces. The inclusion

z-Parameter	Contribution to σ_Q^2	Isotope	Reaction(s)
P_1	91.7%	H-1 in HDPE	(n,el), (n,γ)
P_2	6.1%	C-nat in Graphite	(n,el), (n,in), (n,α)
P_3	1.0%	H-1 in HDPE	(n,el), (n,γ)
P_4	0.6%	H-1 in HDPE	(n,el), (n,γ)

TABLE II. Relative contribution to the total variance and physical meaning of each of the four important independent parameters. Here (n,el) refers to elastic scattering and (n,in) refers to inelastic scattering.

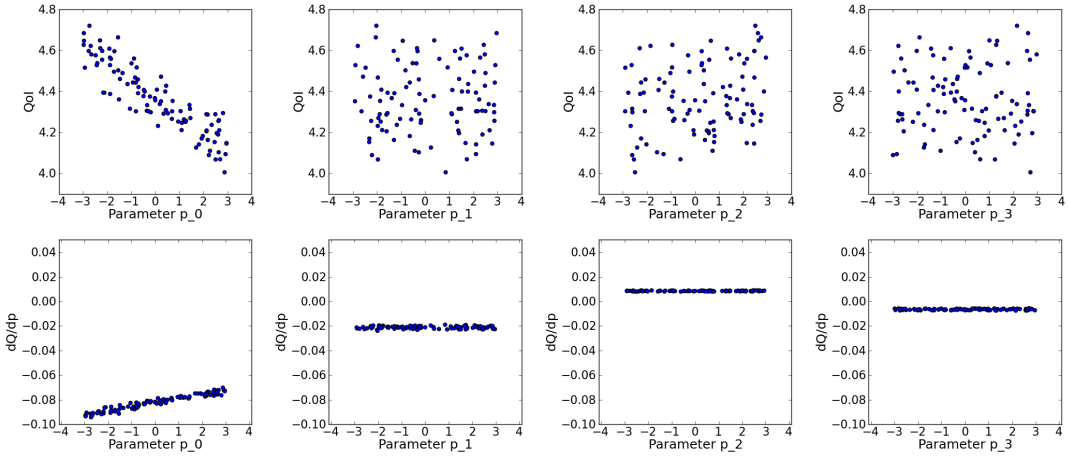

Fig. 1. QoI and partial derivatives of the QoI with respect to the four most important parameters for the IM-1 problem. Each data point represents one forward or adjoint-sensitivity calculation performed at a point drawn randomly from uniform distributions of all of the independent parameters over the domain $[-3, 3]$ and plotted as a function of one parameter at a time.

of derivative information in the gradient-enhanced models appears to slightly accelerate the convergence of the PCE and GPM models, although this effect is not pronounced for this problem. The GE-GPM model demonstrated some instability in the standard deviation between about 75 and 90 data points that was not present in the GPM model.

As the GPM and PCE models are essentially free to construct when compared to the cost of solving the forward and adjoint transport problems it is worth constructing both the point-only and gradient-enhanced models for comparison. As the derivative information was calculated for use in the dimension reduction analysis it may be included in these models at no additional cost, so even minor improvement in surrogate model convergence is beneficial. The oscillations in the GE-GPM model for standard deviation with large numbers of sample points may indicate that the GPM model is more stable without gradient information for this problem.

The QoI calculated at the mean value of the cross sections very closely matches the QoI as calculated with the surrogate models constructed with large pools of data points. This means that a single evaluation of the forward transport problem yields an accurate prediction of the mean value of the QoI for this problem. The standard deviation of the QoI, as estimated by a first-order sensitivity analysis performed at the mean value of the cross sections, similarly matched the standard deviations calculated from the surrogate models with a large number of data points. This result should be unsurprising given second row of plots in Figure (1); that is, three of the four important parameters have partial derivatives that are approximately constant over their range, and the fourth (and most important) parameter's derivative varies slowly and approximately linearly over its range. The fundamental assumption of the first-order sensitivity analysis that the sensitivity coefficients are constant over the input space is nearly satisfied. For this particular problem, then, this analysis suggests that a single forward and single adjoint calculation provide excellent estimates of the QoI and the uncertainty in the QoI.

VII. CONCLUSIONS

The dimension-reduction scheme introduced in this work was demonstrated to identify a very small subset of independent, unit-normal parameters which account for most of the uncertainty in a quantity of interest due to uncertain cross-section data. These parameters capture the correlations present in the nuclear data and are selected based on both the uncertainty in the parameters and the sensitivity of the QoI to these parameters. The original dimensionality of the problem of interest precluded the construction of a surrogate model, but the small subset of important dimensions allowed a variety of response surfaces to be constructed and analyzed. This dimension-reduction technique shows great promise for uncertainty quantification analysis of radiation transport problems with uncertain nuclear data.

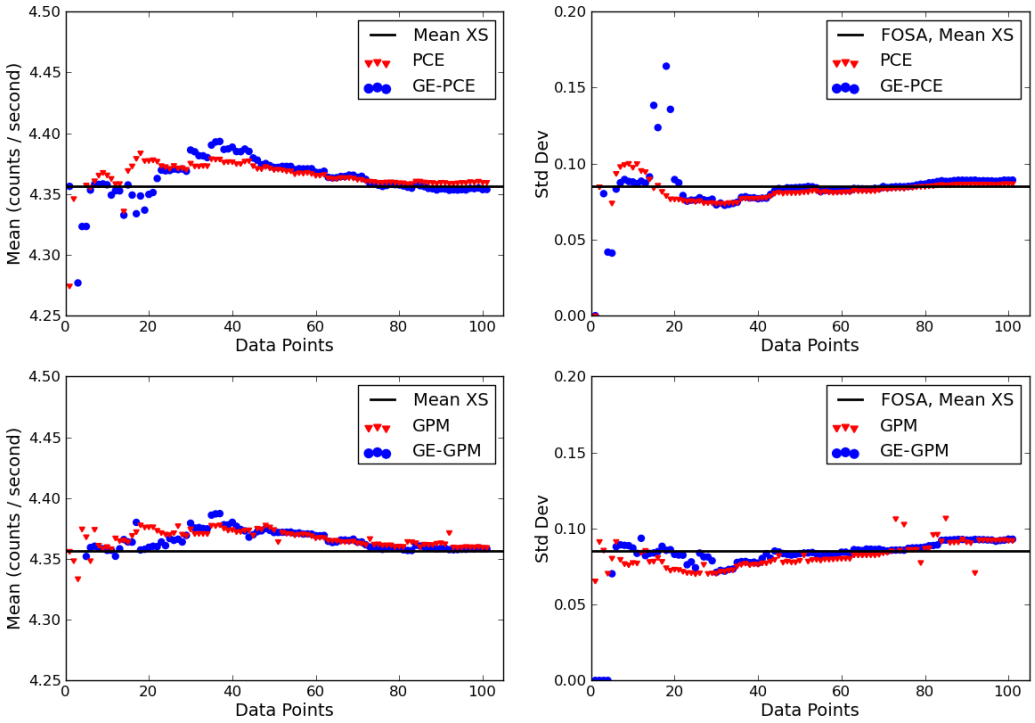

Fig. 2. Mean and Standard Deviation for the CERT Problem as calculated with Dakota using Gaussian process models (top row) and polynomial chaos expansions (bottom row).

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