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GPT-Free Sensitivity Analysis for Monte Carlo Models

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Abstract — *This paper extends the applicability of the generalized perturbation theory (GPT)–free methodology, earlier developed for deterministic models, to Monte Carlo stochastic models. The objective of the GPT-free method is to calculate nuclear data sensitivity coefficients for generalized responses without solving the GPT response-specific inhomogeneous adjoint eigenvalue problem. The GPT-free methodology requires the capability to generate the eigenvalue sensitivity coefficients. This capability is readily available in several of the state-of-the-art Monte Carlo codes. The eigenvalue sensitivity coefficients are sampled using a statistical approach to construct a subspace of small dimension that is subsequently sampled for sensitivity information using a forward sensitivity analysis. A boiling water reactor assembly model is developed using the Oak Ridge National Laboratory Monte Carlo code KENO to demonstrate the application of the GPT-free methodology in Monte Carlo models. The response variations estimated by the GPT-free agree with the exact variations calculated by direct forward perturbations. The GPT-free method is also implemented in OpenMC and tested with the Godiva model to show its capability and feasibility in the estimation of the energy-dependent sensitivity coefficients for generalized responses in Monte Carlo models. The sensitivity results are compared against the ones acquired by the standard GPT-based methodologies. A higher order of accuracy in the sensitivity estimation is observed in the GPT-free method.*

Keywords — *Sensitivity analysis, general perturbation theory–free, Monte Carlo, OpenMC.*

Note — *Some figures may be in color only in the electronic version.*

I. INTRODUCTION

Perturbation theory has attracted the interest of many engineering practitioners because it allows one to estimate the variation in a select model's output, often referred to as response, resulting from a perturbation in the model's input parameters without having to re-execute the model. This provides an invaluable analysis tool since many engineering analyses such as design optimization, surrogate models construction, and uncertainty propagation, etc., require repeated model execution which is typically overwhelming for most realistic engineering models.

The term "generalized" has been coined and primarily used in the nuclear engineering community to differentiate between two different types of responses important to reactor analysis. These responses can be calculated following the solution of the radiation transport model and cast as an eigenvalue problem [see Eq. (1) in Sec. II] for the critical eigenvalue and the flux. If the response of interest is the eigenvalue, one solves the adjoint form of the forward eigenvalue problem [see Eq. (2) in Sec. II] for the so-called fundamental adjoint flux, or simply adjoint flux, which can be subsequently used in conjunction with the forward flux to estimate the eigenvalue variation resulting from general parameter perturbations. For all other responses representing functions of the flux, e.g., reaction rates or reaction rates ratio,

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the term generalized is used to describe the use of perturbation theory. In this case, the adjoint eigenvalue problem has to be solved again with an inhomogeneous source term related to the response of interest. Performing the generalized perturbation theory (GPT) implies the solution of this inhomogeneous equation for the so-called generalized adjoint flux, which can be used in conjunction with the forward flux and the fundamental adjoint flux to estimate the respective response variations.

In the past few decades, the GPT has been widely used to perform sensitivity analysis (SA) for radiation transport models in support of uncertainty quantification, data assimilation, and design optimization applications.[1–5] In our context, a SA is a mathematical procedure used to estimate the derivatives of the model responses with respect to the model's input parameters.[a]

Because it can calculate a given response variation resulting from general parameter perturbations, the GPT is considered computationally superior to forward SA when the number of responses of interest is relatively small compared to the number of input parameters.[b]

However, when the number of responses is large, the GPT becomes computationally taxing due to the large number of adjoint calculations needed. This is because each response of interest requires one generalized adjoint flux.

To implement the GPT approach in a deterministic neutronics model, one needs first to formulate the adjoint model; the mathematical dual of the forward model. Both the forward and the adjoint models can be described as eigenvalue problems. For generalized responses, e.g., a reaction rate at a certain location in the problem domain, one needs to solve the adjoint model in both homogeneous and inhomogeneous forms for the purpose of overcoming the fundamental mode contamination issue in GPT theory.[1,2] Once the adjoint and forward solutions are completed, the calculation of the sensitivity coefficients is considered computationally inexpensive and straightforward (via simple inner product relations) when compared to the cost of obtaining the forward and adjoint solutions.

For stochastically modeled systems such as the Monte Carlo–based neutronics model, three notable approaches have been developed to calculate the sensitivity coefficients, i.e., the first-order derivatives of a response with respect to the group cross sections. The first approach emulates the process adopted by the deterministic approach, but employs a Monte Carlo model to simulate particle transport. For the forward eigenvalue problem, the flux solution can be described by tallies that count the number of particles populating in the various cells in the problem domain. For the homogeneous adjoint eigenvalue problem, a Monte Carlo model simulates particles' importance which can be shown to be equivalent to the adjoint flux.[2] This approach however is limited to the calculation of the sensitivities of the eigenvalue only. The second approach[6] allows one to calculate adjoint-weighted tallies without running a separate adjoint calculation by adapting the iterated fission probability (IFP) technique to the forward eigenvalue calculation. In this approach, one can show that the magnitude of the adjoint flux is directly proportional to the contribution of the particle to the response of interest in a long timescale, which implies the particle's importance to the response. Therefore, the adjoint flux can be accurately estimated in a forward continuous-energy Monte Carlo simulation without an extra overhead to construct the adjoint operator. In nuclear applications whereby responses of interest are integrals of adjoint-weighted quantities, such as kinetics parameters and reactivity changes, the IFP approach has proven to be effective.[6] The third approach, the Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Track length importance CHaracterization, or CLUTCH method,[7] was recently developed by Oak Ridge National Laboratory and implemented in the SCALE code package. Instead of accumulating the contribution of the forward particle during some future generations, the CLUTCH method determines the particle's importance by examining the number of fission neutrons created by that particle based on the predetermination of the adjoint fission source function or importance function in a given spatial mesh. The intriguing point about the CLUTCH method is that it can be readily extended to the GPT framework, which enables the computation of generalized sensitivity coefficients for general responses such as reaction rate ratios. However, the implementation of the CLUTCH method requires knowledge of the generalized adjoint fission source function, which is not known a priori. More importantly, the CLUTCH method quickly becomes computationally expensive when the number of responses becomes large owing to the dual influences of the GPT and Monte Carlo particle simulation.

Our goal on this subject is to devise a new approach that enables Monte Carlo models to calculate the sensitivity coefficients of generalized responses without the need to

[a] For a more general definition of SA, see Saltelli's book.[5]

[b] In forward SA, the forward model must be executed at least n times, where n in the number of input parameters. In each execution, one of the parameters is perturbed and the associated sensitivity coefficients for the perturbed parameter are calculated using the finite differencing approach. Other variations of this approach exist, however the cost is always proportional to n.

determine the generalized adjoint flux and by relying only on the fundamental adjoint solution. The GPT-free methodology has been shown to achieve this goal in deterministic models.[8] This is possibly because the GPT-free depends on an algorithm from randomized matrix theory referred to as the range finding algorithm (RFA). This algorithm takes advantage of the correlation inherent in the simulation between the various responses by identifying the so-called active subspace in the input parameters–space. The active subspace comprises all parameter variations that impact all of the model's responses of interest. The implication is that there exist many directions in the parameter-space that are orthogonal to the active subspace that do not impact the responses. This subspace can be identified by calculating the derivatives of a pseudo response, which is a function of all of the model's responses. The k_{eff} is shown to be an ideal pseudo response because it involves all the flux values everywhere in the combined spatial and energy phase-space. Earlier results of the application of the GPT-free methodology to deterministic models have shown that the size of the active subspace is extremely small compared to the size of the input parameters and responses-spaces. The implication is that one could justify the use of forward SA thereby precluding the need to set up the GPT equations. This paper extends this idea to Monte Carlo models. Furthermore, a comprehensive description of the GPT-free methodology is provided here that builds upon the initial description given in Ref. 8 to develop the so-called "kappa-metric" used to select the size of the active subspace.

Development of an efficient SA for Monte Carlo models is an important and relevant objective given the increased reliance on Monte Carlo models as viable alternatives to deterministic methods for completing reactor physics design and analysis calculations. This is because Monte Carlo methods provide more flexibility for complex reactor geometries and can use the pointwise cross sections directly precluding the need for characteristic of deterministic methods and error-prone group collapsing and homogenization procedures. By tracing the history of each individual particle, the Monte Carlo method predicts the exact path of that particle and calculates many useful quantities of interest by averaging over a very large number of particle histories. Tracking millions to billions of particles is now considered possible given the startling growth in computer power over the past couple of decades. For a GPT-based SA, Monte Carlo methods suffer from two major drawbacks:

1. The execution time is too long to render the repeated execution of the model as required by SA computationally feasible.

2. The statistical variations resulting from the inherent randomness of the simulation must be accounted for in order to differentiate them from the response variations resulting from parameter perturbations.

These limitations motivate the current work to extend the GPT-free methodology to Monte Carlo models. The primary goal of this extension is to preclude the need for a generalized adjoint capability, reduce the computational overhead required when repeated execution of the models is needed, and most importantly, retain an acceptable level of accuracy when compared to the results of existing GPT theory.

The paper is organized as follows. Section II provides a brief overview of GPT theory as applied to deterministic models and highlights the limitations circumvented by the GPT-free methodology. Section III reveals the theory behind the GPT-free methodology and the implementations in Monte Carlo models. Section IV presents a couple of test examples to demonstrate the feasibility and capabilities of the GPT-free method in Monte Carlo applications. The first example is a boiling water reactor (BWR) assembly model with the KENO-V.a code, part of the SCALE (Ref. 9) software package. The second example is the Godiva model developed in OpenMC (Ref. 10). For the sake of a complete discussion, some of the numerical results presented in recent American Nuclear Society venues[11–13] are repeated here before presenting the new results of the current work. Section V concludes the discussion and offers remarks about future work on the GPT-free method applications.

II. GPT BACKGROUND

When applied to calculate the sensitivities of a general response using a deterministic model, the GPT approach requires the solution of an inhomogeneous eigenvalue problem representing the adjoint of the forward eigenvalue problem. The inhomogeneous term depends on the response of interest. The sensitivities of the response could then be determined as a function of the forward and the generalized adjoint flux using simple inner product relations. Mathematically, this procedure may be described with Eqs. (1) and (2):

$$(\mathbf{L} - \lambda\mathbf{F})\phi = 0 \tag{1}$$

and

$$(\mathbf{L}^* - \lambda\mathbf{F}^*)\Gamma^* = g \ , \tag{2}$$

where

$\mathbf{L}$ ($\mathbf{L}^*$), $\mathbf{F}$ ($\mathbf{F}^*$) = forward (adjoint) loss and production operators

λ = eigenvalue (also $\lambda = 1/k$, where k is multiplication factor, or as hereinafter called, the k eigenvalue)

ϕ = forward flux

Γ^* = generalized adjoint flux associated with the inhomogeneous term g that depends on the specific response of interest.

If the eigenvalue represents the response of interest, g is zero, which reduces Eq. (2) to a homogeneous eigenvalue problem:

$$(\mathbf{L}^* - \lambda\mathbf{F}^*)\phi^* = 0 \ , \tag{3}$$

where in this case, the adjoint solution ϕ^* is referred to as the fundamental adjoint flux, and the sensitivity coefficients are then given by[c]

$$\frac{\partial\lambda}{\partial\sigma_i} = \frac{\left\langle \phi^* \left(\frac{\partial\mathbf{L}}{\partial\sigma_i} - \lambda\frac{\partial\mathbf{F}}{\partial\sigma_i} \right)\phi \right\rangle}{\langle \phi^*\mathbf{F}\phi \rangle} \ . \tag{4}$$

The GPT employs a generalized response as a bilinear ratio of the flux solution which can be used to describe many responses of interest, e.g., homogenized few-group cross sections, spectral indices, etc.:

$$R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle} \ . \tag{5}$$

One can show that g in Eq. (2) is given by

$$g = \frac{\partial R}{\partial\phi} = \frac{1}{R}\left(\frac{\Sigma_1}{\langle \Sigma_1, \phi \rangle} - \frac{\Sigma_2}{\langle \Sigma_2, \phi \rangle} \right) \ . \tag{6}$$

The sensitivity coefficients can be determined using inner product relations of the form:

$$\frac{\partial R}{\partial\sigma_i} = R\left[\frac{1}{\langle \Sigma_1, \phi \rangle}\left\langle \frac{\partial\Sigma_1}{\partial\sigma_i}, \phi \right\rangle - \frac{1}{\langle \Sigma_2, \phi \rangle}\left\langle \frac{\partial\Sigma_2}{\partial\sigma_i}, \phi \right\rangle - \left\langle \Gamma^*, \left(\frac{\partial\mathbf{L}}{\partial\sigma_i} - \lambda\frac{\partial\mathbf{L}}{\partial\sigma_i} \right)\phi \right\rangle \right] \ . \tag{7}$$

Since the operator in Eq. (2) is singular, one cannot solve for the generalized adjoint without first solving for the fundamental adjoint from Eq. (2). This is because the so-called fundamental mode decontamination[d] strategy is needed to iteratively remove, via inner product relations, the component of the fundamental adjoint from the generalized adjoint,[1,2] otherwise convergence will not be reached. In deterministic models, if the model is capable of solving the fundamental adjoint equation, it often takes little effort to extend it to solve for the generalized adjoint. The computational cost however is often two to six times more expensive than solving the forward or the fundamental adjoint problem.[14]

For Monte Carlo models, the situation is a little different. As described earlier, the solutions to Eqs. (1) and (2) can be simulated by one of two approaches. In the first approach, one employs Monte Carlo to track the particles and their importance maps in the various regions in the phase-space. These quantities can be used to estimate the forward and adjoint flux, which allows one to calculate the sensitivities of the eigenvalue as done in Eq. (4); see TSUNAMI-3D (Ref. 15) for an example of such an approach. In an alternative approach, it has been shown recently that one could bypass the solution of the fundamental adjoint flux and calculate directly the sensitivity coefficients of the eigenvalue.[6] As described in Sec. I, this approach interprets the adjoint flux as the iteration fission possibility and enables the rigorous estimation of adjoint-weighting factors in continuous-energy Monte Carlo k-eigenvalue calculations. Based on this interpretation, the sensitivity coefficient, if it is in the form of integrals of adjoint-weight quantities, can be obtained via the extension of the general adjoint-weighted tally methods, which can be described as follows:

$$T = \frac{1}{N}\sum_p \pi_p\omega_p \ , \tag{8}$$

[c] Both notations $\langle a, b \rangle = a^T b$ have appeared in nuclear engineering literature to denote the inner product between two vectors (discrete case) or two functionals (continuous case). They will be used interchangeably throughout the text.

[d] The solution of generalized adjoint flux typically contains fundamental homogeneous adjoint flux, and thus the fundamental mode decontamination process is usually performed on the converged solution to remove this component to obtain the pure generalized adjoint flux solution.

where

N = total source weight of generations in the simulation

ω_p = original generation contributions of generalized tally scores (such as reaction rates or ratio of two reaction rates)

π_p = track-length estimator in the final generation population that can be used to estimate the importance function.

Unlike the deterministic world, calculating the adjoint flux appears to be a nontrivial task in Monte Carlo models as it is not clear how a Monte Carlo model could be used to simulate the fundamental mode decontamination, which is easily accomplished in a deterministic model via a Gram-Schmidt orthogonalization strategy.[16]

III. GPT-FREE METHODOLOGY

Recently, the GPT-free methodology has been introduced as an alternative approach for the traditional GPT approach described in Sec. II (Ref. 8). The idea is that instead of calculating directly the sensitivities of the response of interest, the algorithm begins by establishing the so-called pseudo response, which is a general function of the state solution, i.e., the flux for radiation transport problems. The pseudo response attempts to identify the minimum number of degrees of freedom required to describe all possible flux variations, which directly impacts the degrees of freedom available in any set of user-selected responses. Many studies[17–19] have shown that the flux solution exhibits a high degree of correlation between its components. The GPT-free takes advantage of this observation by defining a pseudo response that allows one to estimate the so-called active subspace in the parameters-space. This is done by selecting the eigenvalue as a pseudo response and sampling the eigenvalue sensitivity coefficients at random points in the input parameters-space. This can be achieved by re-evaluating the fundamental adjoint multiple times with different input parameter perturbations. The resulting sensitivity coefficients, with each model execution producing a vector of sensitivities, are aggregated in a matrix which is later processed using a rank revealing decomposition to determine the effective size of the active parameters-subspace. Previous work[8] has shown that the size of the active parameters-subspace is much less than the number of original parameters. This allows one to employ a forward SA to determine sensitivity coefficients for all responses of interest, thereby avoiding the use of Eq. (3). This capability has been demonstrated for deterministic models. In Sec. III, we recall some of these developments and explain their extension to Monte Carlo models.

The GPT-free methodology starts with the observation that any generalized response, e.g., reaction rate in a given region (space and/or energy) in the flux phase-space, can be expressed as a function of the flux and the input parameters, i.e., cross sections:

$$R_i = R_i(\sigma, \phi), \; i = 1, 2, \cdots, m \; . \tag{9}$$

In this representation, m is the total number of responses of interest in the problem, and ϕ is a vector of all flux in terms of all variables in the phase-space, including energy and spacial variables. In reality, local responses depend only on few of these flux values, but the above representation in Eq. (9) is meant to be general. The k eigenvalue describes the neutron balance in the core represented as a ratio of the neutron production and loss terms, which are both functions of the flux values and the cross sections:

$$k = k(\sigma, \phi) \; . \tag{10}$$

Note that unlike the responses, the eigenvalue depends on the flux values everywhere in the phase-space, implying that every single neutron contributes to the multiplication of the system. The responses however could be localized in space and/or energy. Therefore, k may be implicitly related to all generalized responses of interest, described mathematically by

$$k = k(R_1, \cdots, R_m) \; . \tag{11}$$

Through the chain rule of differentiation, it is easy to show that the derivative of k with respect to cross sections, compactly referred to as the k sensitivity vector (or profile), is a linear combination of all responses' sensitivity vectors, i.e.,

$$\frac{dk}{d\sigma} = \sum_{i=1}^{m} \frac{\partial k}{\partial R_i} \frac{dR_i}{d\sigma} \; . \tag{12}$$

The elements of the vector $dk/d\sigma$ represent the first-order derivatives of k with respect to cross sections (commonly referred to as sensitivity coefficients). Similarly, the vector $dR_i/d\sigma$ contains the sensitivity coefficients for the i'th response, and dk/dR_i is a scalar quantity representing the derivative of k with respect to the i'th response, which is expected to be a function of cross sections, composition, geometry, etc. The group cross sections are described by

a vector of length n, i.e., $\sigma \in \mathbb{R}^n$. Second, the gradient calculus definition, which is the direction of maximum response change, basically implies here that parameter perturbations that are orthogonal to the sensitivity vector, i.e., gradient, will produce locally zero response variations. Now, consider the subspace $\mathbb{Z}$ described by

$$\mathbb{Z} = \text{span}\left\{\frac{dR_1}{d\sigma}, \frac{dR_2}{d\sigma}, \cdots, \frac{dR_m}{d\sigma}\right\} \in \mathbb{R}^n \quad . \tag{13}$$

This subspace spans all vectors in the parameter-space that can be described as linear combinations of the unknown responses sensitivity vectors. In reality, the subspace $\mathbb{Z}$ can be considered as a reduced order model (ROM) of the forward model, which in theory can be constructed by many methods with different degrees of approximation.

Implied by Eq. (12), the eigenvalue sensitivity vector belongs to the subspace $\mathbb{Z}$. The dimension of this subspace r can be as large as the dimension of the parameter-space n. However, it has been observed that in most realistic models r is much smaller than n (Refs. 17 and 20). The calculus definition for the gradient then implies that any parameter perturbations that are orthogonal to this subspace will be orthogonal to all responses sensitivity vectors as well as the k-eigenvalue sensitivity vector, and hence, are expected to produce zero response variations. If $r < n$, the implication is that there are $n - r$ directions in the parameter-space that produce zero variations in the responses of interest. Therefore, if the number of responses in a problem becomes large, the GPT-free method outperforms the GPT method because the GPT-free method essentially follows the pathway of the forward method. Furthermore, if the dimension of the subspace r is small and one can readily identify the subspace $\mathbb{Z}$, a forward SA could be employed instead of a GPT approach to calculate responses sensitivities. In this case, the effective number of input parameters is reduced to r, and hence, the computational cost will be proportional to r rather than n. This represents the basic philosophy behind the GPT-free methodology.

It is important to note that in practice whenever cross sections are varied, the responses are expected to change. In our context, zero response change implies that the change is negligibly small. Therefore, it is important that the user defines the accuracy sought for the sensitivities which is used by the GPT-free algorithm to determine the appropriate size r of the subspace $\mathbb{Z}$. Moreover, an error analysis ensuring that all sensitivities are estimated within the user-defined accuracy must be carried out.

The subspace $\mathbb{Z}$ estimated via the so-called RFA, the error analysis resulting from restricting parameter perturbations to the subspace, and finally, the forward SA to determine responses sensitivities, are detailed in Secs. III.A, III.B, and III.C.

III.A. Estimation of the GPT-Free Subspace $\mathbb{Z}$

Returning to the definition in Eq. (13), form a symbolic matrix which contains the m responses sensitivity vectors as columns:

$$\mathbf{B} = \left[\frac{dR_1}{d\sigma}, \frac{dR_2}{d\sigma} \cdots \frac{dR_m}{d\sigma}\right] \in \mathbb{R}^{n \times m} \quad . \tag{14}$$

These columns are not known a priori, thus assume that the matrix is available in an abstract form only. As described earlier, to complete the forward SA, the GPT-free algorithm requires the determination of the subspace $\mathbb{Z}$. From linear algebra, this subspace represents the mathematical range of the matrix $\mathbf{B}$, i.e., $\text{R}(\mathbf{B}) = \mathbb{Z}$, which is defined as follows:

$$\text{R}(\mathbf{B}) = \{q; \text{ such that } q = \mathbf{B}\chi \text{ for all } \chi \in \mathbb{R}^m\} \quad . \tag{15}$$

This definition describes the set of vectors that can be generated by all possible linear combinations of the columns of the matrix $\mathbf{B}$. In past work, an RFA was introduced that employs only matrix products with random vectors.[20] In an article appearing in the applied mathematics community,[21] rigorous error bounds were developed for this algorithm. The computational cost is $r + s$ random matrix-vector products, where r is the expected rank of the matrix and s are additional oversamples employed to ensure the user-defined error tolerance is achieved.

Introducing the RFA, employing Eq. (12), and defining $\chi \in \mathbb{R}^m$ as an m-tuples vector whose i'th component is given by $\chi_i = \partial k / \partial R_i$, one can rewrite the k-eigenvalue sensitivity vector as follows:

$$\frac{dk}{d\sigma} = \mathbf{B}\chi \quad , \tag{16}$$

where $\chi \in \mathbb{R}^m$ is an m-tuples vector whose i'th component is given by $\chi_i = \partial k / \partial R_i$. Equation (16) implies that the evaluation of the k-eigenvalue sensitivity vector is equivalent to performing a matrix-vector product involving the unknown matrix $\mathbf{B}$. This process could be repeated as many times as needed with different parameter perturbations to emulate the effect of randomized matrix-vector product as required by the RFA mentioned above. The implication is that the k-eigenvalue sensitivity vector is a vector that lives in the subspace $\mathbb{Z}$. By creating

different snapshots of that vector, each created with randomized parameter perturbations, one can span the entire subspace $\mathbb{Z}$. The use of random numbers is required by the RFA. It ensures that the first r matrix-vector products are independent, and hence, can be employed to form a basis for the subspace. Assuming $\mathbb{Z}$ has dimension r, all additional matrix-vector products become linearly dependent on the first r vectors. This helps trigger a termination point for the RFA. For more details on the theory and history of RFAs, Refs. 21 and 22 are highly recommended.

As employed by the GPT-free methodology, the RFA is described as follows:

1. Estimate initial dimension r, and let $r' = r$.
2. Generate r' cross-section perturbations represented by $\{\Delta\sigma\}_{i=1}^{r'}$
3. Generate t more cross-section perturbations, and let $r' = r' + t$
4. Employ the available methodology to evaluate the sensitivity coefficients of the eigenvalue and form the matrix $\mathbf{Z} = \left\{\frac{dk}{d\sigma}\right\}_{i=1}^{r'} \in \mathbb{R}^{n\times r}$
5. Calculate the QR decomposition $\mathbf{Z} = \mathbf{QR}$
6. Generate j random cross-section perturbations $\{\Delta\sigma\}_{i=1}^{j}$, where j is determined from Wilks' formula.[23]
7. Calculate the components $\{\Delta\sigma^{\perp}\}_{i=1}^{j}$ of the cross-section perturbations in step 4 that are orthogonal to the range of $\mathbf{Z}^T$ via $\Delta\sigma_i^{\perp} = \left(\mathbf{I} - \mathbf{QQ}^T\right)\Delta\sigma_i$, $i = 1, 2, \cdots, j$
8. Execute the forward model j times using the orthogonal perturbations from step 7, and record the responses variations
9. Test the κ-metric (which is described in Sec. III.B), if the user-defined error criterion is not met, return to step 3; otherwise the range r is set to be r'
10. END

In the current implementation, the input perturbations in step 2 comprise cross-section perturbations only, but in general one could include other types of input parameter perturbations such as isotopic concentration, geometry, etc., when one is interested in getting the sensitivity coefficients for a wider range of conditions, e.g., overdepletion, different spectral conditions, etc.

III.B. GPT-Free Error Analysis (κ-Metric Definition)

Employing the results from Sec. III.A, the subspace $\mathbb{Z}$ may be described by a set of basis vectors as follows:

$$\mathbb{Z} = \text{span}\{q_1, q_2, \cdots, q_j\} \in \mathbb{R}^n \ .$$

Now consider any general input parameter (i.e., cross sections) perturbation, one can write:

$$\Delta\sigma = \Delta\sigma^{\parallel} + \Delta\sigma^{\perp} \ , \tag{17}$$

where

$$\Delta\sigma^{\parallel} = \left(\sum_{i=1}^{r} q_i q_i^T\right)\Delta\sigma$$

and

$$\Delta\sigma^{\perp} = \left(\mathbf{I} - \sum_{i=1}^{r} q_i q_i^T\right)\Delta\sigma \ .$$

A graphic interpretation of the projections given in Eq. (17) is illustrated in Fig. 1.

The basic premise of the GPT-free methodology is that a perturbation orthogonal to the subspace $\mathbb{Z}$, such as the component $\Delta\sigma^{\perp}$, does not change (within user-defined accuracy) the responses of interest. This means

$$\left|R_i(\sigma_0 + \Delta\sigma) - R_i\left(\sigma_0 + \Delta\sigma^{\parallel}\right)\right| \le \varepsilon, \ i = 1, 2, \cdots, m \ . \tag{18}$$

To ensure the credibility of the GPT-free results, this premise must be carefully assessed using an error analysis. This is facilitated by employing an order statistics–type metric, referred to hereinafter as the κ-metric,[20] calculated to ensure Eq. (18) is satisfied for all responses.

The κ-metric is based on Wilks' order statistics, where one can assign a confidence for the measure in

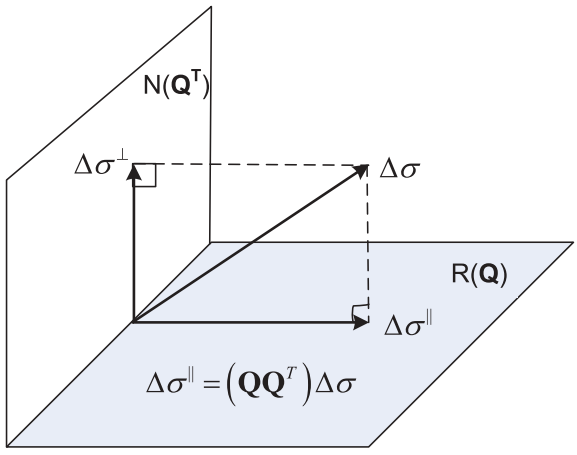

Fig. 1. Projection of Δσ onto the subspace $\mathbb{Z}$.

Eq. (18) due to j samples and a probability p (Ref. 23). The required number of samples j can be determined from the Wilks' formula:

$$\left(1-p^{j}\right)-j(1-p)p^{j-1}\geq c\ , \tag{19}$$

where p is the probability and c is the confidence. Using this definition, if jp of the j samples meets the error tolerance in Eq. (18) then the accuracy of the determined subspace is acceptable with confidence c.

The specific form of the κ-metric should be application dependent, i.e., determined by the user to meet the needs of the analysis. Below are some examples. Equation (20) calculates the absolute error for the i'th response resulting from the discarding of the orthogonal component:

$$\kappa_i=\left|R_i(\sigma_0+\Delta\sigma)-R_i\left(\sigma_0+\Delta\sigma^{||}\right)\right|\ . \tag{20}$$

Equation (21) calculates a single κ-metric as the root-mean-square absolute error for a group of responses of the same type, e.g., flux distribution:

$$\kappa=\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left|R_i(\sigma_0+\Delta\sigma)-R_i(\sigma_0+\Delta\sigma^{||})\right|^2}\ . \tag{21}$$

Equation (22) duplicates Eq. (21) but in a relative sense:

$$\kappa=\frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left|R_i(\sigma_0+\Delta\sigma)-R_i(\sigma_0+\Delta\sigma^{||})\right|^2}}{\frac{1}{N}\sum_{i=1}^{N}\left|R_i(\sigma_0)\right|}\ . \tag{22}$$

Note however that all responses are normalized by the same value; in this example, the average reference response:

$$\kappa=\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left|\frac{R_i(\sigma_0+\Delta\sigma)-R_i(\sigma_0+\Delta\sigma^{||})}{R_i(\sigma_0)}\right|^2}\ . \tag{23}$$

One can also calculate the root mean square for the relative error calculated for each response where the normalization is response dependent. This error metric choice is typically unfavorable because it amplifies the effect of large relative errors for responses whose absolute values are negligibly small.

III.C. GPT-Free Forward SA

This subsection describes how the sensitivity coefficients for the responses of interest are calculated once the subspace is identified and the error analysis is completed. Recall the responses equation:

$$R_i=R_i(\sigma,\phi)\ . \tag{24}$$

Since the flux and the cross sections are related by the forward model, i.e., the flux is determined based on the input cross sections, one can write the response as a function of the cross sections only:

$$R_i=R_i(\sigma)\ . \tag{25}$$

The previous discussion implies that the response calculated with a general cross-section perturbation $\Delta\sigma$ can be approximated by

$$R_i=R_i\left(\sigma_0+\Delta\sigma^{||}\right)\ , \tag{26}$$

where $\Delta\sigma^{||}=\mathbf{Q}\mathbf{Q}^T\Delta\sigma$. This implies that in general $\Delta\sigma^{||}$ has nonzero components along the r columns of the matrix $\mathbf{Q}$, which may be expressed as

$$\Delta\sigma^{||}=\sum_{i=1}^{r}\alpha_i q_i\ , \tag{27}$$

where $\alpha_i=q_i^T\Delta\sigma^{||}$ is the component of $\Delta\sigma^{||}$ along q_i. One can then rewrite the response equation as

$$R_i=R_i\left(\sigma_0+\sum_{i=1}^{r}\alpha_i q_i\right)\ \text{or}\ R_i(\alpha_1,\alpha_2,\cdots,\alpha_r)\,. \tag{28}$$

Equation (28) implies that any general response depends on r-reduced input parameters, which represent the components of a general cross-section perturbation along the $\{q_i\}_{i=1}^{r}$ vectors. If r is a small number, one can employ finite differencing to calculate the sensitivities of the responses with respect to these reduced parameters. These sensitivities can then be folded back in terms of the original parameters. One important advantage of this approach is that it allows one to evaluate higher-order derivatives if nonlinear behavior is of interest. Higher-order derivatives are expensive to obtain if the number of input parameters is very large. This will be investigated in future work.

First, the forward SA may be executed as follows:

1. FOR $j = 1, \cdots, r$
2. Pick a scalar perturbation $\Delta\alpha_j$
3. Calculate $\Delta R_i = R_i(\sigma_0 + \Delta\alpha_j q_j) - R_i(\sigma_0)$ for all responses of interest.
4. END

Assuming the perturbations are within the linear range, one can approximate ΔR_i as follows:

$$\Delta R_i \simeq \frac{\partial R_i}{\partial \alpha_j} \times \Delta\alpha_j \quad . \tag{29}$$

Using the chain rule of differentiation:

$$\frac{dR_i}{d\sigma} = \frac{dR_i}{d\alpha}\frac{d\alpha}{d\sigma} = \sum_{j=1}^{r} \frac{\partial R_i}{\partial \alpha_j}\frac{d\alpha_j}{d\sigma} = \mathbf{Q}\frac{dR_i}{d\alpha} \quad . \tag{30}$$

IV. NUMERICAL EXAMPLES

IV.A. BWR Assembly Model

A BWR 10 × 10 lattice model is studied serving as the first test example for the application of the GPT-free methodology. The model is originally developed for the Monte Carlo code MCNP (Ref. 24) and has been converted for the TSUNAMI-3D (Ref. 15) sequence in the SCALE code package.[9] The multigroup Monte Carlo–based KENO-V.a module in TSUNAMI-3D sequence solves for both the fundamental forward and adjoint fluxes which are subsequently used by the SAMS module to calculate the sensitivities of the k eigenvalue. SAMS employs traditional perturbation theory approach to calculate the first-order derivatives of k with respect to cross sections.

The BWR assembly, depicted in Fig. 2, consists of 91 fuel pins laid over a 10 × 10 grid with a square-shaped coolant channel in the middle of the assembly. The assembly employs UO_2 nuclear fuels with seven different ^{235}U enrichments. The dimensional quantities for the major components in the assembly are summarized in Table I.

To measure the efficiency of the GPT-free methodology in a general scenario when all isotopes and their associated reaction types are included, the initial model is depleted over a 365-day cycle and the fuel compositions at the middle of the cycle are taken to represent the model. The compositional inventory is represented by seven types of UO_2 nuclear fuels with different ^{235}U weight percent enrichments and fission product compositions.

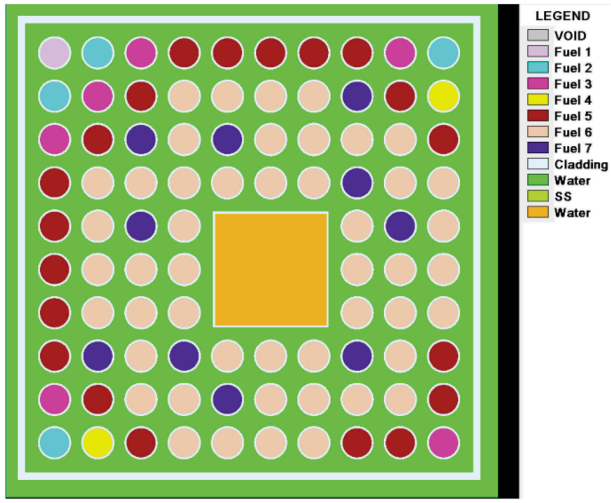

Fig. 2. Schematic view of the BWR assembly.

TABLE I

Dimensions of Major Components in the Assembly

Component	Dimension	
Assembly	Length	13.400 cm
	Boundary	13.860 cm
Water hole	Length	1.295 cm
Fuel pin	Pellet diameter	0.867 cm
	Cladding inner	0.884 cm
	Cladding outer	1.005 cm
	Pitch	1.295 cm

In this preliminary study, the average fission spectrum χ_g, the fission and capture cross sections of nine fissionable nuclides, and the capture cross sections of 14 notable fission products are considered as input parameters whose sensitivities are to be calculated. Using a 238-energy-group structure for seven different mixtures, the total number of input parameters is $(3 \times 9 + 14) \times 238 \times 7 = 68\,306$. The reference eigenvalue is given by $k = 1.0723 \pm 0.0001$. Note that the statistical uncertainty is in the order of 10 pcm of $\Delta k/k$. This error represents deviations in the k due to the statistical nature of Monte Carlo calculations, and it is therefore reasonable to expect the same level of discrepancy for the GPT-free results. In the application of larger practice problems, a looser convergence criterion (such as an order of 100 pcm for $\Delta k/k$) could be used for the subspace development to save computation cost, but the tolerance of the κ-metric has to be adjusted accordingly, which will inevitably degrade

the accuracy of the GPT-free model. Thus a trade-off study is needed to balance the efficiency and accuracy of the method.

In this study, the sensitivity coefficients for k are calculated via a traditional perturbation theory approach which combines the fundamental solutions for the forward and adjoint eigenvalue problem. This is done by the SAMS sensitivity evaluation module. It is worthwhile to note here that in general the GPT-free methodology does not restrict the manner by which the first-order derivatives are calculated. It however requires that one have access to a capability that generates first-order derivatives for k at user-defined input cross-section values.

The GPT-free employs a RFA approach to construct the Z subspace.[21,25,26] The algorithm has been described in detail in Sec. III and is briefly re-iterated here:

1. Randomly perturb cross sections $\sigma_{\text{pert},i} = \sigma_0 + \Delta\sigma_i$
2. Execute the SA sequence in SCALE to calculate $dk/d\sigma|_i$
3. Repeat r times and form the decomposition:

$$\mathbf{QR} = [\, dk/d\sigma|_1 \quad \cdots \quad dk/d\sigma|_r \,] \in \mathbb{R}^{n\times r}$$

4. Evaluate the κ-metric; increase r until error is below user-defined tolerance.

The κ-metric for the k-eigenvalue changes with the increase of dimension of the subspace in this study is shown in Fig. 3.

Here the κ-metric is defined as the form of

$$\kappa = \left| k_{\text{pert}} - k_{\text{app}} \right| \ , \tag{31}$$

where k_{pert} represents the exact value for k due to a general cross-section perturbation and k_{app} represents the GPT-free approximation, resulting from restricting the cross-section perturbations to the GPT-free subspace. The cross-section perturbations associated with each case is given by:

$$\sigma_{\text{pert}} \ = \ \sigma_0 + \Delta\sigma \tag{32}$$

and

$$\sigma_{\text{app}} = \sigma_0 + \left(\mathbf{QQ}^T\right)\Delta\sigma \ .$$

The results indicate that the error initially declines with increasing the dimension of the subspace. The rate of error decline decreases and a plateau behavior develops starting at approximately r = 619, which is two orders of magnitude smaller than the original number of input parameters, n = 68 306. Note that the minimum error reached is about 10 pcm, which is of the same order of magnitude of the statistical uncertainty in the estimated k value.

The κ-metric for the thermal flux is shown in Fig. 4 as the dimension of the subspace is increased. The plots in Fig. 4 exhibit the same behavior as Fig. 3 does as a function of the dimension of the subspace. From the reference case, the statistical error of the thermal flux averages at 0.038%. The plots in Fig. 4 show that the

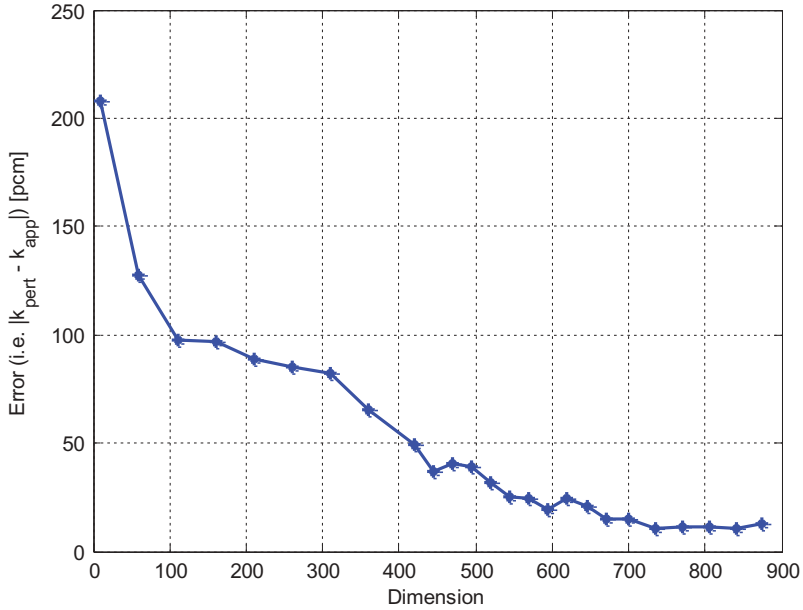

Fig. 3. The κ-metric for the eigenvalue.

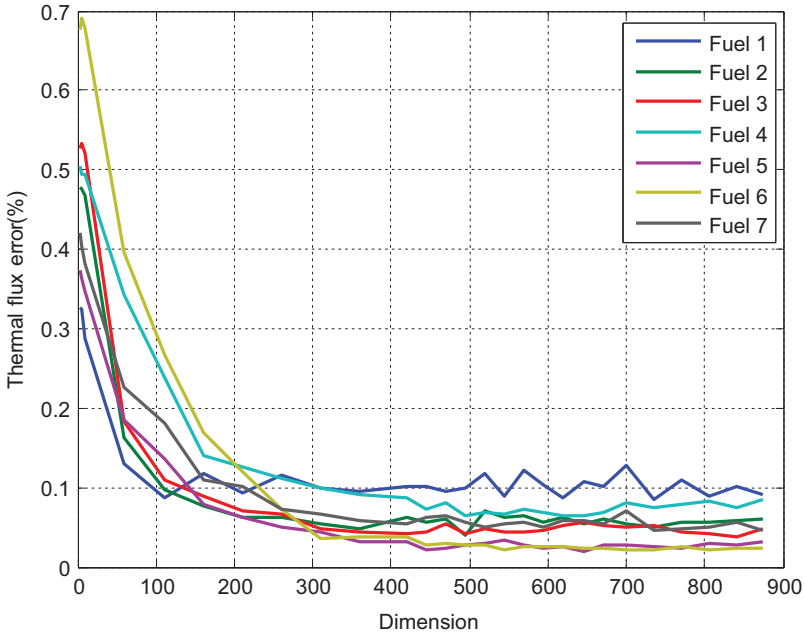

Fig. 4. The κ-metric for the thermal flux in fuels.

κ-metric plateaus at the level of statistical uncertainty, with a minimum rank of $r = 619$ in this study.

To quantify the discrepancies between the GPT-free estimated and exact responses, 30 cases are employed with random cross-section perturbations, and the respective response variations are compared. Figure 5 demonstrates the results of the study for the eigenvalue as a response.

The eigenvalue discrepancy is shown in per cent mille. Each of the blue dots represents the exact variation in the eigenvalue due to a given random cross-section perturbation. The red circles represent the κ-metric, that is the discrepancy between the GPT-free estimate and the exact variation for each case calculated with a rank $r = 619$. i.e., $|k_{\text{pert}} - k_{\text{app}}|$, the cross sections associated with k_{pert} and k_{app} are described in Eq. (32). The results show that the discrepancies are in the order of 10 to 50 pcm, which is the same order of magnitude of the statistical uncertainty of reference calculations.

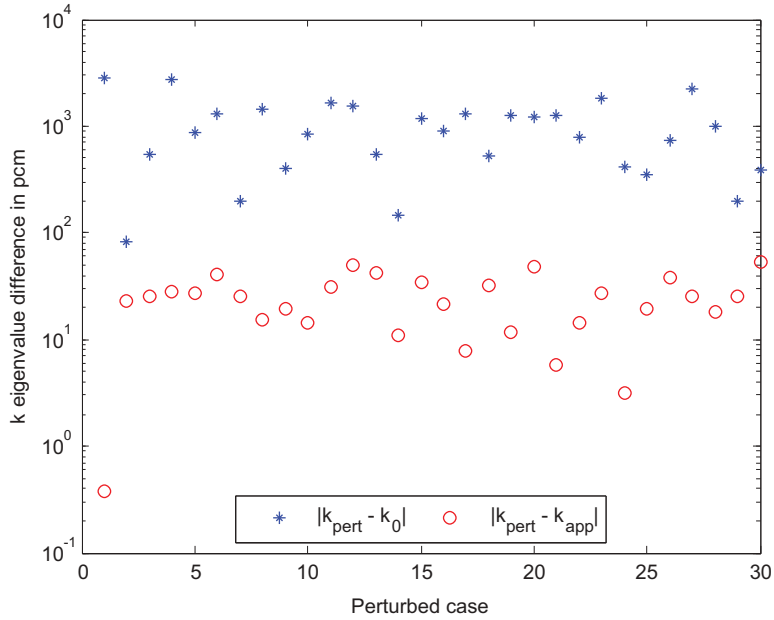

Fig. 5. The GPT-free errors for k eigenvalue.

To check the adequacy of the subspace to capture generalized responses, the thermal flux values in different pins are employed as responses. Figure 6 shows the thermal flux discrepancy errors for a representative pin for each of the 30 cases studied. The variations on the y-axis are normalized to the average thermal flux value.

Similarly, the blue stars display the exact variations, and the red circles describe the discrepancies. The results indicate that the discrepancies are consistently low and of the same order of magnitude as the statistical error of thermal flux from the forward calculations averaging at 0.038%. It is worthy of mentioning that both the differences in Fig. 6 and the statistical error of thermal flux are measured in a relative sense to the averaged thermal flux in the reference calculations, that is $err = \frac{\sigma_{\Phi^T}}{\Phi_0^T}$.

IV.B. Godiva Model

Godiva, a fast-spectrum criticality benchmark problem model, is used as a second test bed for the application of the GPT-free method in Monte Carlo models. Godiva is a bare metallic sphere of highly enriched (94 wt%) uranium. The Godiva sphere benchmark contains isotopes ^{234}U,^{235}U, and ^{238}U, and has a radius 8.74 cm. OpenMC (Ref. 10) is adopted as the Monte Carlo tool to analyze the Godiva model in this paper because continuous-energy SA capabilities were recently developed in OpenMC (Ref. 27) with a combination of IFP method[6] and CLUTCH methods,[7] which enables OpenMC to calculate sensitivity coefficients for both the k eigenvalue and generalized responses (e.g., reaction rate ratios) via the conventional GPT methodologies popularized in the deterministic transport community.[1–5] This makes OpenMC an ideal tool for assessing the efficacy of the GPT-free method in estimating nuclear data sensitivity coefficients.

To assess the GPT-free method, the IFP module in OpenMC is used to calculate k-eigenvalue sensitivity with respect to the fission cross section of ^{235}U while the CLUTCH-FM module is used to calculate sensitivities of a generalized response of interest. Without loss of generality, a generalized response function considered in this work is defined as

$$R = \frac{\Sigma_f^{238}\mathrm{U}\phi}{\Sigma_f^{235}\mathrm{U}\phi} \quad , \tag{33}$$

namely, the ratio of integrated fission reaction rates of two fissionable nuclides, ^{235}U and ^{238}U. This quantity is of interest in determining the fast neutron utilization factor, one of the important factors in the famous four-factor formula used to estimate the neutron multiplication factor of a reactor. This quantity is also very useful to justify the unique and strong feature of the GPT-free method on responses that cannot be efficiently handled by the GPT approach because it involves individual reaction rate, flux, etc. The standard SCALE 44-energy-group structure[28] is utilized in the perturbation and sensitivity profile calculations, while the 300 K ENDF/B-VII.1

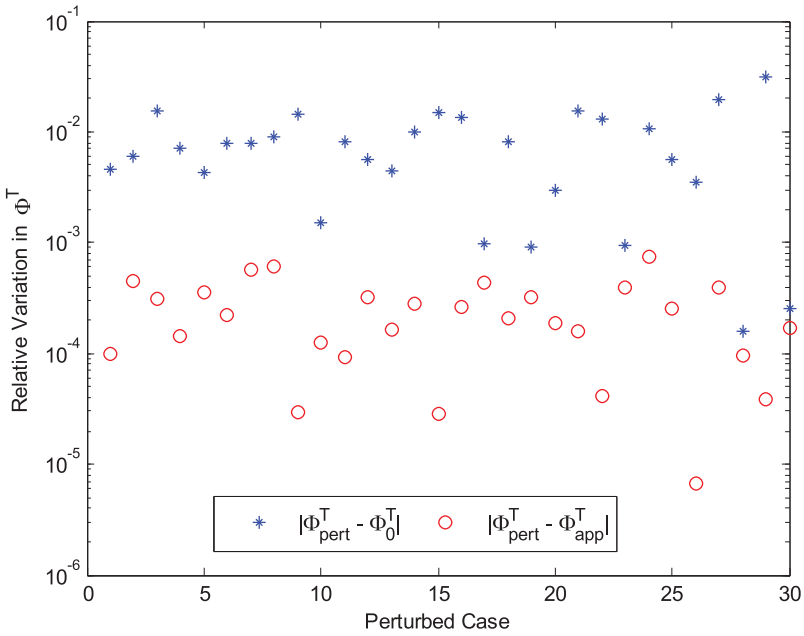

Fig. 6. The GPT-free errors for thermal flux.

library is used as the input neutron cross-section data for OpenMC simulation.

The standard GPT-free algorithm applied to the above BWR assembly model in KENO is performed on the Godiva model with similar steps implemented in OpenMC. The cross-section perturbations in this example are achieved by adding noise to the fission cross section of ^{235}U in each group following a Gaussian distribution with a relative standard deviation of 2% (larger deviations are also tested in the model and the same effect on the results is noticed). These randomly perturbed cross sections are employed to perform k-sensitivity calculations using OpenMC. The characteristic subspace matrix of the sensitivities can be constructed from the energy-groupwise k-sensitivity coefficients, followed by identifying a subspace or ROM through QR decomposition of the subspace matrix.

Following the RFA in Ref. 23 a reduced rank of $r = 12$ is estimated to limit the associated errors in the k eigenvalue resulting from the ROM model. If the ROM model and its associated rank are selected appropriately, the discarded components should have negligible impact on the estimated k eigenvalue and other responses of interest. Figure 7 shows the results of an example comparing the ROM model predictions to 50 direct perturbations without any reduction. The circle (red) and plus (blue) symbols in Fig. 7 represent the changes of the k_{eff} value in the two perturbed conditions, respectively, while the cross signs show their differences. It is noteworthy to mention that the statistical errors caused by the Monte Carlo simulation were purposely controlled to be negligibly small in all calculations performed in this study to ensure no cross contamination of the ROM construction process.

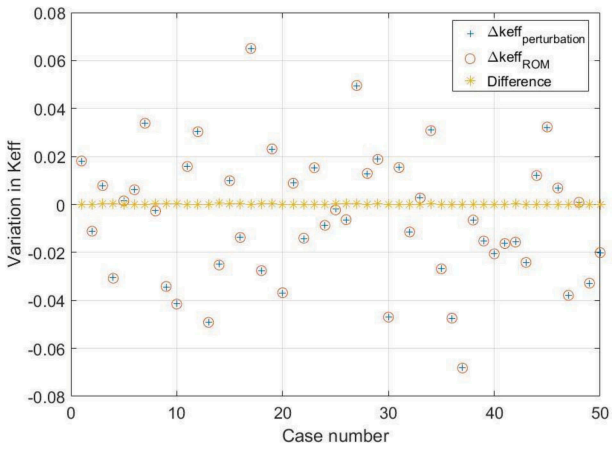

Fig. 7. Validation of ROM with k perturbations.

As seen in Fig. 7, the variations of the k_{eff} value for the ROM case accurately approximates the one in the direct perturbation case. The implication is that a ROM with an effective rank nearly captures the dominant directions of cross-section variations.

Next, the sensitivity of a generalized response R was estimated using the GPT-free theory. A new N set of randomly generated cross-section perturbations was generated, and the forward model was executed N times using OpenMC to determine the variations of the response as follows:

$$\Delta R_i = R(\vec{\sigma}_0 + \Delta\vec{\sigma}_i) - R(\vec{\sigma}_0),\ i = 1, \cdots, N\ . \tag{34}$$

The response sensitivity can then be evaluated by

$$\frac{dR}{d\vec{\sigma}} = \mathbf{Q}_r(\mathbf{\Gamma}^T)^{\dagger}\Delta\vec{\mathbf{R}}\ , \tag{35}$$

where

$$\mathbf{\Gamma} = [\vec{\gamma}_1, \cdots, \vec{\gamma}_K], \vec{\gamma}_i = \mathbf{Q}_r^T\Delta\vec{\sigma}_i,\ i = 1, \cdots, N\ . \tag{36}$$

For comparison, the same response sensitivity was calculated using the GPT module developed in OpenMC. Figure 8 illustrates the 44-groupwise sensitivity coefficients obtained from the two approaches. Note the response sensitivities shown in Fig. 8 have been transformed into a dimensionless form, i.e., $(dR/R)/(d\vec{\sigma}/\vec{\sigma})$, and presented as sensitivity per unit lethargy rather than energy. As seen in Fig. 8, the two groupwise sensitivity coefficient curves yielded by the OpenMC GPT capability and the GPT-free method agree quite well. Relative larger discrepancies are exhibited in higher energies, which is meaningful as Godiva is a criticality benchmark operated under fast-spectrum conditions.

Alternatively, the performance of the GPT-free method can be assessed using the variation of response. To demonstrate it, we generated another 50 randomly generated cross-section perturbations. The perturbed responses are first tallied using forward calculations for reference. In the same time, the response sensitivities obtained from both the GPT and GPT-free approaches are used to predict the response variations described as follows:

$$\Delta R_{\mathrm{SA}} = \left(\frac{dR}{d\vec{\sigma}}\right)^T \cdot \Delta\vec{\sigma}\ , \tag{37}$$

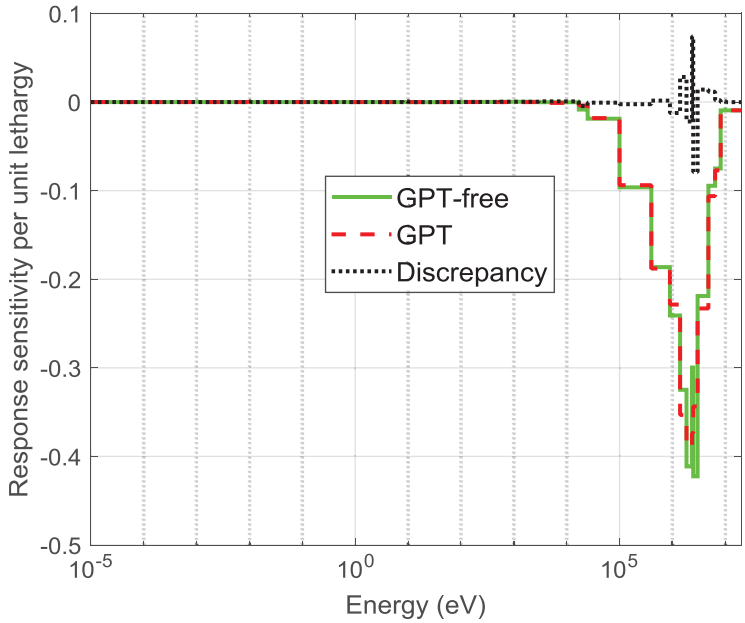

Fig. 8. Comparison of groupwise sensitivity coefficients by the GPT and GPT-free.

where $dR/d\vec{\sigma}$ was again obtained by Eq. (35). The results of the three approaches described above are plotted in Fig. 9, in which the plus and asterisk symbols describe the absolute errors of predicted response variations using the GPT-free and GPT approaches, respectively. Figure 9, consistent with Fig. 8, verifies that both approaches estimate response sensitivity accurately.

It is also observed in Fig. 9 that the GPT-free results are even closer to the reference perturbation values as compared to the GPT method. This can be explained by the following two facts. First, the traditional GPT approach calculates response variations using first-order approximations, implying that nonlinear variations are discarded. Second, the RFA employed to construct the ROM model is based on sampling of the k-sensitivity vector. The implication is that the active subspace will capture directions responsible for nonlinear behavior because if the model is perfectly linear, the k-sensitivity vector will not change. This reveals one of the key features of the GPT-free: It is capable of identifying an active subspace that captures both linear and nonlinear variations. Therefore, if coupled with an effective forward-based SA, e.g., variance-based decomposition, it can be used to capture nonlinear variations in a computationally efficient manner.

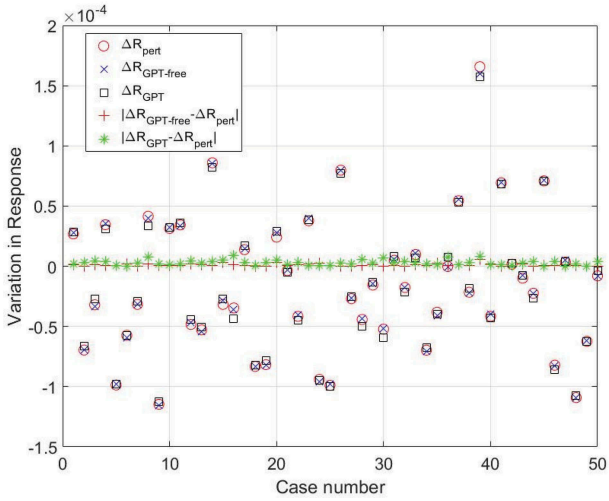

Fig. 9. The GPT-free accuracy for response variations.

V. CONCLUSIONS

The GPT-free methodology is successfully applied to a Monte Carlo BWR assembly model and Godiva model to perform SA of generalized responses with respect to cross sections representing the input parameters to the model. A ROM is employed to significantly reduce the effective number of input parameters in order to enable a forward SA, thereby precluding the need to set up the conventional GPT inhomogeneous eigenvalue problem. The algorithm requires access to the sensitivities of the k eigenvalue only and employs elements from linear algebra to find the so-called active subspace which describes the effective input parameters.

Ongoing work focuses on extending this methodology to include depletion effects for deterministic models as

well as Monte Carlo models to replace the traditional depletion perturbation theory (DPT) developed in the nuclear engineering community.[29] The DPT is computationally much more demanding than the GPT, especially when done for realistic reactor models. To our knowledge, there is currently no implementation of the DPT in any of the commercial or publicly available codes. Our goal is to render the DPT computationally feasible by eliminating the need to solve the inhomogeneous eigenvalue problem backward in time. Moreover, we continue to investigate other approaches to further reduce the cost of constructing the active subspace. Recent results indicate that one to two orders of magnitude reduction in the computational cost is possible, which we believe is essential to render the approach more attractive for routine design calculations.

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