Application of GPT-Free Method to Sensitivity Analysis in Monte Carlo Models

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INTRODUCTION

Generalized perturbation theory (GPT) has been widely applied to sensitivity analysis of engineering systems models for decades. It is proven to be an efficient tool to calculate sensitivities in various applications such as uncertainty quantification, adaptive simulation and design optimization [1-3]. GPT is computationally advantageous when the number of responses of interest is relatively small compared to the number of input parameters. However, in applications where both the number of input parameters and output responses become significantly large, GPT can become computationally intractable due to the considerable number of adjoint calculations needed. In addition, for engineering systems that are modeled stochastically, e.g., the Monte-Carlo particle transport model commonly used in reactor analysis benchmark calculation, there currently exist no general extensions of GPT theory.

To enable sensitivity analysis of generalized responses in Monte-Carlo models, the GPT-free method, recently developed for deterministic models [4], is employed. GPT-free is based on the idea that the eigenvalue is implicitly dependent on all generalized responses, representing functionals of the flux vector. This implies that the sensitivities of generalized responses with respect to cross-sections can be linearly related to eigenvalue sensitivities. A reduced order model based on subspace theory employs first order derivatives of the eigenvalue with respect to cross-sections, sampled at random cross-sections values, to identify a subspace. This subspace is subsequently explored for sensitivity information for generalized responses using forward sensitivity analysis approach. This precludes the need to construct the response-specific inhomogeneous adjoint equation as required by GPT theory. This salient feature of the GPT-free method makes it particularly suitable for sensitivity analysis application in large scale models, where the construction of GPT equations is either infeasible or impractical.

Ref. [4] provides details on the GPT-free theory and demonstrates its application to deterministic radiation transport models. This summary describes recent efforts to extend the applicability of GPT-free method to Monte Carlo models. As proof of principle, the method is demonstrated using a Monte Carlo EPR assembly model.

GPT-FREE METHODOLOGY

The idea of GPT-free is based on the following two observations. First, any generalized response, e.g. reaction rate in a given region (space and energy[1]) in the flux phase space, can be expressed as a function of the flux vector. Similarly, the k eigenvalue (or simply k) represents a ratio of the neutron production and loss terms which are both functions of the flux values everywhere in the phase space. Therefore, k may be implicitly related to all generalized responses of interest, described mathematically by:

$$k = k(R_1, \cdots, R_m) \tag{1}$$

Here $\{R_i\}$ may be thought of as a set of elementary responses, from which any other response can be derived. Elementary responses represent the microscopic reaction rates for all nuclides calculated at all regions in the flux phase space[2]. If the GPT-free approach allows one to calculate these elementary responses, then any generalized response of interest could be readily calculated. 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.

$$\frac{dk}{d\bar{\sigma}} = \sum_{i=1}^{m} \frac{\partial k}{\partial R_i} \frac{dR_i}{d\bar{\sigma}} \tag{2}$$

The elements of the vector $dk/d\bar{\sigma}$ represent the first order derivatives of k with respect to cross-sections (commonly referred to as sensitivity coefficients). Similarly, the vector $dR_i/d\bar{\sigma}$ 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 cross-sections are described by a vector of length n, $\bar{\sigma} \in \mathbb{R}^n$.

Second, recalling the definition of the gradient from calculus, the sensitivity vector for a given response is the

[1] The time dependence will be treated in future work.

[2] In reality, these elementary responses will not be calculated; they are only employed abstractly to derive the GPT-free theory.

direction in the cross-sections space that results in the maximum response change. Perturbations in cross-sections that are orthogonal to the sensitivity vector will produce zero first order variations in the response.

Now returning to the representation in Eq.(2), the implication is that the k sensitivity vector belongs to the subspace spanned by the responses sensitivity vectors. If this subspace is known a priori and has a small dimension r, that is much smaller than the dimension of the cross-sections space n, one can perform a forward sensitivity analysis excluding all cross-sections perturbations that are orthogonal to the subspace. This results in reducing the effective dimensionality of the model, and thereby the computational cost of forward sensitivity analysis. In Ref. [4], it is shown that by evaluating the k sensitivity vector with random cross-sections perturbations, this subspace can be identified.

To assess the quality of the subspace, an error metric is developed as follows: let $\mathbb{N}$ denote the subspace determined by the GPT-free method. Let $\mathbf{Q}$ be an orthonormal matrix of rank r whose columns span the subspace $\mathbb{N}$. Let $\Delta\bar{\sigma}$ represent an arbitrary cross-section perturbation, which may be decomposed into two orthogonal components as follows [5]:

$$\Delta\bar{\sigma} = \Delta\bar{\sigma}^{\parallel} + \Delta\bar{\sigma}^{\perp}, \qquad (3)$$

where the components $\Delta\bar{\sigma}^{\parallel}$ and $\Delta\bar{\sigma}^{\perp}$ represent, respectively, the component of cross-sections perturbation that is parallel and orthogonal to the GPT-free subspace. If the subspace $\mathbb{N}$ is known as a priori, one can calculate $\Delta\bar{\sigma}^{\parallel}$ via projection theory [5] as follows

$$\Delta\bar{\sigma}^{\parallel} = \left(\mathbf{Q}\mathbf{Q}^{T}\right)\Delta\bar{\sigma}. \qquad (4)$$

This projection operation is illustrated in Fig. 1.

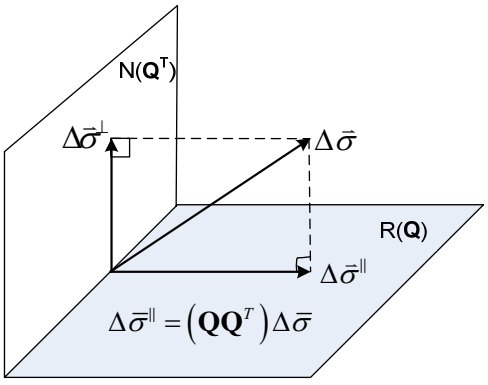

Fig. 1. The projection of $\Delta\bar{\sigma}$ onto $\mathbb{N}$.

Therefore cross-sections perturbations can be further expressed as:

$$\Delta\bar{\sigma} = \mathbf{Q}\mathbf{Q}^{T}\Delta\bar{\sigma} + \Delta\bar{\sigma}^{\perp}. \qquad (5)$$

By restricting cross-sections perturbations to the subspace only, the implication is that the cross-sections variations orthogonal to the subspace will produce negligible variations in the responses, i.e.

$$\left|R_i\left(\bar{\sigma}_0 + \Delta\bar{\sigma}^{\perp}\right) - R_i\left(\bar{\sigma}_0\right)\right| \le \varepsilon \qquad (6)$$

Eq.(6) describes the basic idea for the κ -metric calculated for all responses of interest in order to assess the performance of the subspace. Moreover, it allows one to estimate the size of the subspace required to meet a user-defined error tolerance. Detailed discussion on the significance of this approach and the statistical meaning of this metric may be found in Ref. [4].

EPR ASSEMBLY MODEL

In this summary, a European Pressurized Reactor (EPR) assembly model is studied serving as a test bed for the application of the GPT-free method. The model is originally developed for the Monte Carlo code MCNP [6] and has been converted for the TSUNAMI-3D [7] sequence in the SCALE code package [8]. The 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.

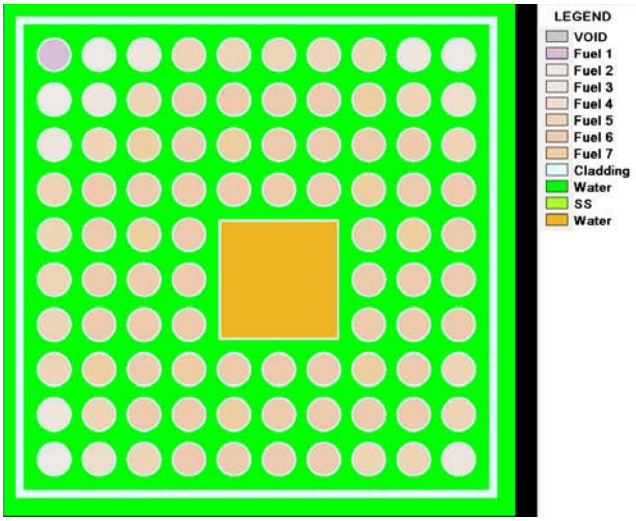

Fig. 2. Schematic view of the EPR assembly.

Note that the GPT-free method does not restrict the manner by which the first order derivatives are calculated. It however requires that one has access to a capability that generates first-order derivatives for k at user-defined input cross-section values.

The EPR assembly, depicted in Fig. 2, consists of 91 fuel pins laid over a 10 x 10 grid with a square-shaped coolant channel in the middle of the assembly. UO_2 nuclear fuels with 7 different U-235 enrichments are employed. In this preliminary study, only the fission and capture cross-sections of the fuel nuclides, including U-235, U-236, U-238, Np-237, Pu-239, Pu-240, Pu-231, are considered as input parameters whose sensitivities are to be calculated. With a 238 energy group structure, the total number of input parameters is 2x7x238 = 3332. The reference eigenvalue is given by: $k = 1.069968 \pm 0.0001$. Note that the statistical uncertainty is in the order of 10 pcm. This error represents deviations in the k due to the statistical nature of Monte Carlo calculations, and is therefore reasonable to expect the same level of discrepancy for the GPT-free results, if the implementation is successful.

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.

GPT-free employs a range finding algorithm approach to construct the subspace [9, 10]. The algorithm is briefly re-iterated here:

1. Randomly perturb cross-sections $\bar{\sigma}_{\text{pert},i} = \bar{\sigma}_0 + \Delta\bar{\sigma}_i$
2. Execute the sensitivity analysis sequence in SCALE to calculate $dk/d\bar{\sigma}\big|_i$
3. Repeat r times and form the decomposition: $\mathbf{QR} = \left[dk/d\bar{\sigma}\big|_1 \quad \ldots \quad dk/d\bar{\sigma}\big|_r \right] \in \mathbb{R}^{n \times r}$
4. Evaluate the κ metric; increase r until error is below user-defined tolerance.

The κ metric for the k eigenvalue is shown in Fig. 3 as the dimension of the subspace is increased. The k_{pert} represents the exact value for k due to a general cross-section perturbation.

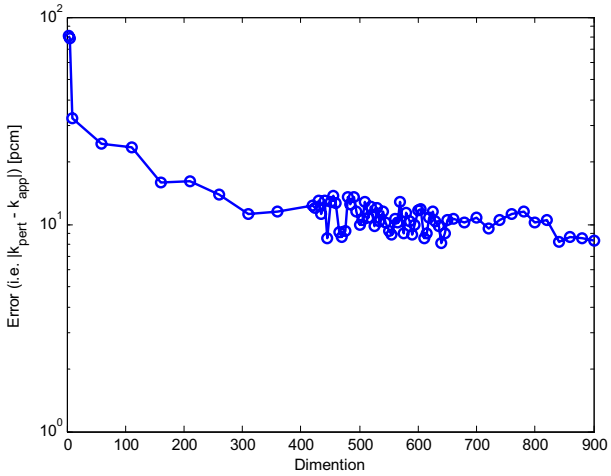

Fig. 3. The κ metric for the eigenvalue.

The 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 both cases are given by:

$$\begin{aligned} \bar{\sigma}_{\text{pert}} &= \bar{\sigma}_0 + \Delta\bar{\sigma} \\ \bar{\sigma}_{\text{app}} &= \bar{\sigma}_0 + \left(\mathbf{Q}\mathbf{Q}^T\right)\Delta\bar{\sigma} \end{aligned} . \qquad (7)$$

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=300. This is one order of magnitude smaller than the number of input cross-sections, n=3332. 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.

To check the adequacy of the subspace to capture generalized responses, the thermal flux values in different pins are employed as responses. Employed are 25 different cases, in each case the cross-sections were randomly perturbed, and the exact variations in the thermal flux values are calculated. The GPT-free theory is then used to calculate an estimate for the flux variations. Fig. 4 shows the thermal flux error for a representative pin for each of the 25 cases studied. The variations on the y-axis are normalized to the average thermal flux value.

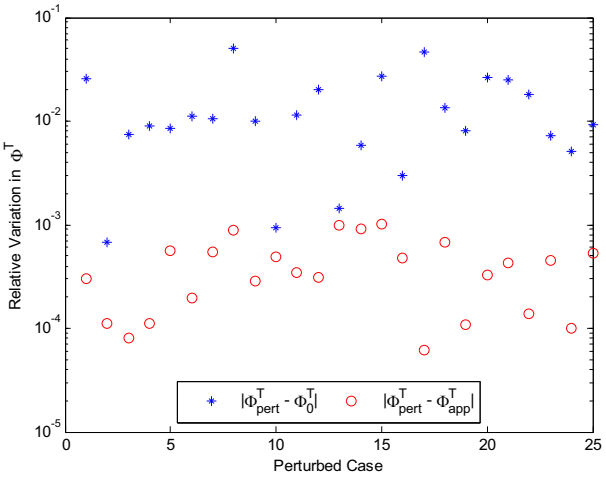

Fig. 4. GPT-free errors for thermal flux.

Errors are consistently low and of the same order of magnitude as the statistical error of forward calculations, which is found to be 0.02%.

CONCLUSIONS

GPT-free method is successfully applied to a Monte Carlo based EPR model to perform sensitivity analysis of generalized responses with respect to cross-sections. A reduced order model is employed to reduce the effective number of cross-sections in order to enable a forward sensitivity analysis; thereby precluding the need for setting up GPT equations. The algorithm requires access to the sensitivities of the *k* eigenvalue only.

Ongoing work is focusing on extending this methodology to include depletion effects for deterministic models. If successful, we will investigate application to Monte Carlo models.

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