Nuclear Data Sensitivity Analysis in OpenMC Using the GPT-Free Method

Jingang Liang,[1] Zeyun Wu,[2]* Hany S. Abdel-Kalik[3]

[1]*Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 USA*
[2]*Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, VA 23219 USA*
[3]*School of Nuclear Engineering, Purdue University, West Lafayette, IN 47907 USA*
**zwu@vcu.edu*

INTRODUCTION

Adjoint-based general perturbation theory (GPT) has been widely used to perform nuclear data (i.e., cross-sections) sensitivity analysis (SA) in reactor physics [1-3]. A general definition of SA may be found in a number of references, see for example Saltelli's definition [4]. In our context, SA is as a mathematical procedure designed to estimate the derivatives of model output responses with respect to the model's input parameters. Because GPT can calculate a given response variation resulting from general parameter perturbations, GPT-based SA is considered computationally superior to forward SA when the number of responses of interest is relatively small compared to the number of input parameters. However, when the number of responses is large, GPT becomes computationally taxing due to the large number of adjoint calculations needed. This follows as one generalized adjoint flux is required for each response of interest.

The goal of the GPT-free method is to devise an approach that enables models to calculate the sensitivities of generalized responses relying only on the eigenvalue sensitivities obtained using the solution of the homogeneous adjoint eigenvalue problem. GPT-free is based on the idea that the eigenvalue is implicitly dependent on all generalized responses, representing functionals of the flux vector, which implies that the sensitivities of generalized responses with respect to cross-sections can be linearly related to eigenvalue sensitivities. In GPT-free method, reducing order modeling (ROM) is employed to identify the so-called active subspace in the input parameters space via random sampling of model's input parameters and re-evaluation of the homogeneous adjoint eigenvalue problem. This subspace is subsequently explored for sensitivity information of generalized responses using forward sensitivity analysis approach. In doing so, GPT-free method precludes the need to construct the response-specific inhomogeneous adjoint equation, referred to as the GPT equations. 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.

The GPT-free method was formerly employed to achieve this goal in deterministic radiation transport models [5] and Monte Carlo models [6, 7]. The application of GPT-free method in deterministic models is quite successful because the sampling of the eigenvalue sensitivity coefficients can be accomplished in a manageable computation time after efficiently reducing the effective dimensionality of the input parameters space. With the reduced dimension being much smaller than the original number of input parameters, one could justify the use of forward SA thereby precluding the need to set up the GPT equations. Earlier work has demonstrated the application of GPT-free to the estimation of generalized response variations [6, 7]. In this summary, we present new results on GPT-free for the estimation of the full energy-dependent sensitivity coefficients for generalized responses. This capability is expected to enable the use Monte Carlo models for a wide range of engineering applications, previously done with deterministic models, e.g., uncertainty quantification and parameter inference.

In the paper, the GPT-free method is implemented and tested with the open-source Monte Carlo code OpenMC [8]. Continuous-energy SA capabilities were recently developed in OpenMC [9]. The combination of iterated fission probability (IFP) and Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Track length importance CHaracterization (CLUTCH) methods 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 deterministic transport community [1-4]. This makes the OpenMC an ideal tool for assessing the efficacy of the GPT-free method in estimating nuclear data induced sensitivity coefficients. In this work, the GPT-free approaches described in Ref. 5 and 6 are applied in an OpenMC model and the energy-dependent response sensitivities are calculated and compared with the results obtained from the OpenMC integrated GPT modules developed upon the IFP and CLUTCH methods.

OVERVIEW OF THE GPT-FREE METHOD

The GPT-free method starts with the assumption that any generalized response can be expressed as a function of the flux and the input parameters, i.e., cross-sections.

$$R_i = R_i\left(\sigma,\ \phi\right),\ i = 1,2,....,m\,, \tag{1}$$

where R_i denotes a general response, σ is cross-sections, and ϕ is a vector of all flux values over the combined phase space of energy, space, and angle. In reactor physics, the *k* eigenvalue describes the neutron balance in a reactor core and is represented as a ratio of the neutron production and loss terms that are both functions of the flux values and the cross-sections, thus *k* can be written as

$$k = k(\sigma, \phi). \quad (2)$$

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:

$$k = k(R_1, \cdots, R_m). \quad (3)$$

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

$$\frac{dk}{d\sigma} = \sum_{i=1}^{m} \frac{\partial k}{\partial R_i} \frac{dR_i}{d\sigma}. \quad (4)$$

The elements of the vector $dk/d\sigma$ represent the first order derivatives of *k* with respect to cross-sections. 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.

Therefore, considering a subspace described by

$$\mathbb{Z} = \text{span}\left\{\frac{dR_1}{d\sigma}, \frac{dR_2}{d\sigma}, ..., \frac{dR_m}{d\sigma}\right\} \in \mathbb{R}^n, \quad (5)$$

where *n* a vector length for the cross-sections, this subspace spans all vectors in the parameter space that can be described as linear combinations of the unknown responses sensitivity vectors. It has been reported repeatedly that in most realistic models the dimension of the subspace *r* is much smaller than the dimension of the cross-sections *n* [10, 11]. The calculus definition of the gradient 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. Hence, if *r* is small and one can easily 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 reveals the basic idea 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 dimension of the active subspace $\mathbb{Z}$. Moreover, an error analysis ensuring that all sensitivities are estimated within the user-defined accuracy must be carried out. The implementation of GPT-free method typically involves three steps: the estimation of the active subspace $\mathbb{Z}$ via the so-called range finding algorithm (RFA); the error analysis resulting from restricting parameter perturbations to the subspace; and finally the forward-based SA to determine response sensitivities.

GPT-FREE APPLICATION IN OPENMC

Godiva, a fast spectrum criticality benchmark problem model, is used as a test bed for the application of GPT-free method in OpenMC. Godiva is a bare metallic sphere of highly enriched (94 wt.%) Uranium. Godiva sphere benchmark contains isotopes ^{234}U, ^{235}U and ^{238}U, and has a radius 8.74 cm. To assess the GPT-free method, the IFP module in OpenMC is used to calculate *k* eigenvalue sensitivity w.r.t 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, the generalized response function considered in this work is defined as Eq. (6), namely a 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. The standard SCALE 44 energy-group structure [12] is utilized in the perturbation and sensitivity profile calculations, while the 300K ENDF/B-VII.1 library is used as the input neutron cross section data for OpenMC simulation.

$$R = \frac{\Sigma_f^{^{238}\text{U}} \phi}{\Sigma_f^{^{235}\text{U}} \phi}. \quad (6)$$

The standard GPT-free algorithm is performed on the Godiva model, with the steps detailed below. Note the cross section perturbations in this work are achieved by adding noise to the fission cross section of ^{235}U in each group from a Gaussian distribution (the relative standard deviation 2%), as described in Eq. (7)

$$\vec{\sigma}_{\text{pert}} = \vec{\sigma}_0 + \Delta\vec{\sigma}, \quad (7)$$

where $\vec{\sigma}_{\text{pert}}$, $\vec{\sigma}_0$, $\Delta\vec{\sigma}$ denote the perturbed cross section, reference cross section and the randomly imposed noise to the base value, respectively.

To proceed, randomly generated cross section perturbations are employed to perform *k*-sensitivity calculations using OpenMC. According to Eq. (5), the

subspace matrix $\mathbb{Z}$ can be constructed from the energy-group-wise *k*-sensitivity coefficients, followed by identifying a subspace or ROM through QR decomposition described in Eq. (8).

$$\mathbb{Z} = \mathbf{Q}_r \mathbf{R}_r, \quad \mathbf{R}_r \in \mathbb{R}^{r\times r} \text{ and } \mathbf{Q}_r \in \mathbb{R}^{n\times r}. \tag{8}$$

Following the RFA in Ref. 12, a reduced rank of $r = 12$ is estimated to limit the associated errors in the *k* eigenvalue resulting from the reduction. This is done via a comparison of variations of *k* eigenvalue with two cross section perturbations, $\Delta\vec{\sigma}$ and $\Delta\vec{\sigma}^{\|}$, which is really $(\mathbf{Q}_r\mathbf{Q}_r^T)\Delta\vec{\sigma}$. The latter represents the component of the cross-section perturbation that belongs to the active subspace, with the remaining component representing the one that is discarded by 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. Fig. 1 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. 1 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.

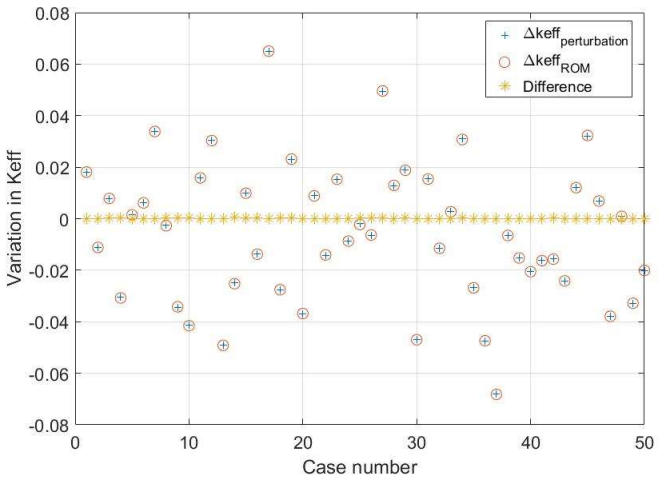

Fig. 1. Validation of ROM with *k* perturbations.

As seen in Fig. 1, the variations of the k_{eff} value for the ROM case accurately approximates the one in the direct perturbation case, which indicates

$$k(\vec{\sigma}_0 + \Delta\vec{\sigma}^{\|}) \approx k(\vec{\sigma}_0 + \Delta\vec{\sigma}). \tag{9}$$

The implication is that an ROM with an effective rank r=12 nearly captures the dominant directions of cross-sections variations.

Next, the sensitivity of a generalized response *R* was estimated using the GPT-free theory [5-7]. We create new *N* set of randomly generated cross sections perturbations, and execute the forward model *N* times using OpenMC and determine the changes in the response as described in Eq. (10).

$$\Delta R_i = R(\vec{\sigma}_0 + \Delta\vec{\sigma}_i) - R(\vec{\sigma}_0),\ i = 1,...,N. \tag{10}$$

The response sensitivity can then be evaluated by

$$\frac{dR}{d\vec{\sigma}} = \mathbf{Q}_r(\mathbf{\Gamma}^T)^{\dagger}\Delta\vec{\mathbf{R}}, \tag{11}$$

where

$$\mathbf{\Gamma} = [\vec{\gamma}_1,...,\vec{\gamma}_K],\ \ \vec{\gamma}_i = \mathbf{Q}_r^T\Delta\vec{\sigma}_i,\ i = 1,...,N. \tag{12}$$

For comparison, the same response sensitivity was calculated using the GPT module developed in OpenMC. Fig. 2 illustrates the 44-group-wise sensitivity coefficients obtained from the two approaches. Note the response sensitivities shown in the figure has been transformed into a dimensionless form (i.e., $(dR/R)/(d\vec{\sigma}/\vec{\sigma})$). As seen in Fig. 2, the two group-wised sensitivity coefficient curves yielded by OpenMC GPT capability and the GPT-free method agree quite well.

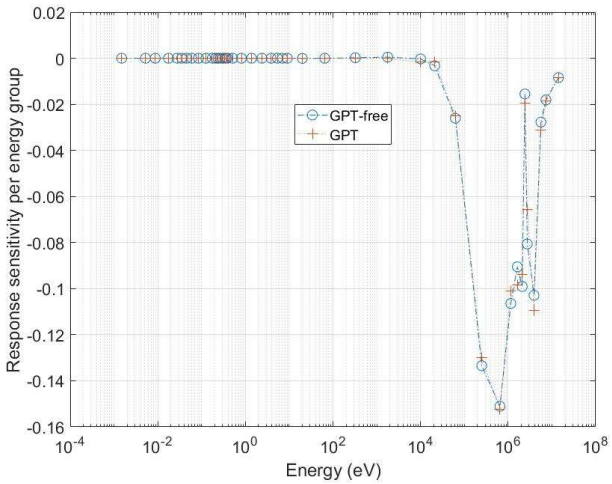

Fig. 1. Comparison of group-wised sensitivity coefficients of a generalized response with GPT and GPT-free.

Alternatively, the performance of the GPT-free method can be assessed using the variation of response. To demonstrate it, we generate another 50 randomly generated cross sections 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 in Eq. (13).

$$\Delta R_{SA} = \left(\frac{dR}{d\vec{\sigma}}\right)^T \cdot \Delta\vec{\sigma}, \tag{13}$$

where $\frac{dR}{d\vec{\sigma}}$ was again obtained by Eq.(11). The results of the three approaches described above are plotted in Fig. 3,

in which the plus and asterisk symbols describe the absolute errors of predicted response variations using GPT-free and GPT approaches respectively. Fig. 3, as consistent to Fig. 2, verifies that both approaches estimate response sensitivity accurately.

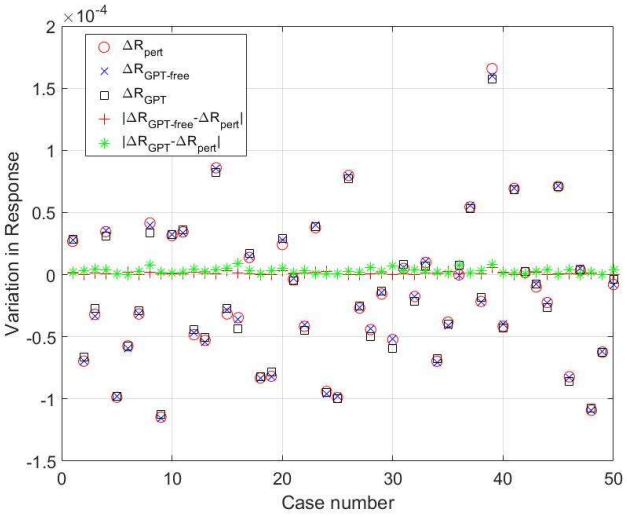

Fig. 2. GPT-free accuracy for response variations.

It is also observed in Fig. 3 that the GPT-free results are even closer to the reference perturbation values as compared to the GPT method. To explain that, we recall two facts. First, the traditional GPT approach calculates response variations using first-order approximations, implying that nonlinear variations are discarded. Second, the range finding algorithm 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 GPT-free that 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.

CONCLUSIONS

This paper summarized recent research efforts to extend the GPT-free method, a computationally efficient method for sensitivity coefficients evaluation, to the OpenMC code. The goal is to enable an efficient computation of sensitivity coefficients when the number of responses is too large to render the GPT approach computationally feasible. GPT-free achieves that by re-casting SA using a forward-based approach with much smaller input space, determined using ROM techniques. The reduced space, denoted active subspace, is selected by sampling the k-sensitivity vector a number of times which allows one to constrain the errors resulting from discarding all input parameters components that are orthogonal to the active subspace. Results indicate the GPT-free methodology is capable of estimating the sensitivity coefficients to the level of accuracy expected by the ROM model, which can be tuned to user-selection. Future work will extend GPT-free work to depletion problems as an alternative to depletion perturbation theory (DPT), which has proven to be even more computationally demanding than GPT, because its cost becomes proportional to the square of the number of time steps required to complete depletion calculations.

REFERENCES

1. M. WILLIAMS, *Handbook of Nuclear Reactor Calculations-Perturbation Theory for Nuclear Reactor Analysis*, CRC Press, III (1986).
2. A. GANDINI, "A Generalized Perturbation Method for Bi-Linear Functionals of the Real and Adjoint Neutron Fluxes," *Journal of Nuclear Energy*, **21**, 755-765 (1967).
3. D. CACUCI, "On the Application of the Adjoint Method of Sensitivity Analysis to Problems in the Atmospheric Sciences," *Atmósfera*, 7, 47-59 (1994).
4. A. SALTELLI, *Sensitivity Analysis in Practice: A Guide to assessing Scientific Models*, John Wiley & Sons (2004).
5. C. KENNEDY, C. RABITI, and H. ABDEL-KHALIK, "GPT-Free Sensitivity Analysis for Eigenvalue Problems", *Nuclear Technology*, 1**79**(2), 169-179 (2012).
6. Z. WU, C. B. KENNEDY, and H.S. ABDEL-KHALIK, "Application of GPT-Free Method to Sensitivity Analysis in Monte Carlo Models," *Trans. Am. Nucl. Soc.*, **106**, 763-766 (2012).
7. Z. WU and H. S. ABDEL-KHALIK, "Further GPT-free Developments for Monte Carlo Models," *Trans. Am. Nucl. Soc.*, **107**, 981-984 (2012).
8. P. K. ROMANO et al., "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development," *Ann. Nucl. Energy*, **82**, 90-97 (2015).
9. X. PENG et al., "Development of continuous-energy sensitivity analysis capability in OpenMC," *Annals of Nuclear Energy*, **110**, 362-383 (2017).
10. Y. BANG, H. ABDEL-KHALIK, and J. HITE, "Hybrid Reduced Order Modeling Applied to Nonlinear Models", *International Journal for Numerical Methods in Engineering*, **91**(9), 929-949 (2012).
11. E. LIBERTY, et al., "Randomized Algorithms for the Low-Rank Approximation of Matrices", *Proceedings of the National Academy of Science*, **104** (2007).
12. S. M. BOWMAN, "SCALE 6: comprehensive nuclear safety analysis code system," *Nuclear technology* **174**(2), 126-148 (2011).