Exact-to-Precision Generalized Perturbation Theory: Analytical Analysis

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INTRODUCTION

Exact-to-Precision Generalized Perturbation Theory (E_PGPT) is the new development in generalized perturbation theory (GPT) that is intended to extend its applicability to estimate higher-order variations in all responses in the model with respect to all possible perturbations in the model's input parameters [1-4]. E_PGPT places high premium on computational efficiency in order to render GPT a standard analysis tool in routine design and safety reactor calculations. This approach was first introduced into reactor physics in 2011 for one-group source-driven problems in diffusion theory [1], and then the theory was further extended to multi-group eigenvalue problems in 2012 [2]. Although, classical GPT has been distinguished as a powerful mathematical tool in sensitivity analysis and uncertainty quantification, it still faces two major obstacles. *First*, to properly capture exact variations (i.e. all higher orders) in the response of interest, the associated number of model executions becomes dependent on either the number of parameters or the number of points in the flux phase space [5, 7]. *Second*, the computational burden of GPT is dependent on the number of responses; this is because a separate adjoint solution is required for each response of interest [6]. For realistic design calculations based on high fidelity multi-scale multi-physics models with large volumes of data manipulated at each code-to-code interface, the number of parameters, responses, and flux phase space points are expected to be very large. These major obstacles arising with classical GPT are overcome via new development in E_PGPT in order to revive the interest in GPT for routine design calculations.

The purpose of this summary is to demonstrate the use of E_PGPT by solving a simple analytic example. Many of the properties discussed in previous work [1, 2] can be illustrated in this manner.

METHODOLOGY

For the sake of a complete discussion, we provide a brief overview of GPT and E_PGPT. The reader is referred to Refs. [1, 6] for the detailed description.

Consider the following time-independent form of Boltzmann equation for neutron transport:

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

where the neutron flux, ϕ, is a function of continuous variables in space, energy, and direction. The **P** operator represents all the terms in the transport equation, the **L** and **F** operators represent neutron loss and fission production, respectively. λ is the smallest eigenvalue (equal to $1/k_{eff}$) associated with the eigenvector ϕ. Note that the normalization of the function ϕ can be chosen arbitrarily since the operator **P** is ill-posed. For simplicity, ϕ is normalized so that its phase-integral is equal to one.

The adjoint criticality equation is:

$$\mathbf{P}^*\phi^* = \left(\mathbf{L}^* - \lambda\mathbf{F}^*\right)\phi^* = 0 \tag{2}$$

The first-order GPT estimation for the variation in λ which results from the perturbation is:

$$\Delta\lambda_{1st} = \frac{\left\langle \phi^*, \left(\Delta\mathbf{L} - \lambda\Delta\mathbf{F}\right)\phi \right\rangle}{\left\langle \phi^*, \mathbf{F}\phi \right\rangle} \tag{3}$$

where the brackets '<>' represent the integration that is carried over the whole accessible range of the variables, and the perturbations in the operators are denoted as $\Delta\mathbf{L}$ and $\Delta\mathbf{F}$.

Higher-order GPT evaluation of variations in the λ have been suggested by Gandini [8] based on expanding the perturbed flux in terms of the λ eigenfunctions of Eq. (2) and iteratively obtaining higher order estimates for the eigenvalue perturbation as follows.

$$\lambda^i = \frac{\left\langle \phi^*, \Delta\mathbf{L}\varphi^{i-1} \right\rangle + \lambda^{i-1}\left\langle \phi^*, \Delta\mathbf{F}\varphi^0 \right\rangle}{\left\langle \phi^*, \mathbf{F}\phi \right\rangle} + \frac{\sum_{j=1}^{i-1}\left\langle \phi^*, \left(\lambda^{i-(j+1)}\Delta\mathbf{F} + \lambda^{i-j}\mathbf{F}\right)\varphi^j \right\rangle}{\left\langle \phi^*, \mathbf{F}\phi \right\rangle} \tag{4}$$

where the λ eigenfunctions can be computed recursively from the equations:

$$
\begin{aligned}
&\left(\mathbf{L}-\lambda^0\mathbf{F}\right)\varphi^0 = 0\\
&\left(\mathbf{L}-\lambda^0\mathbf{F}\right)\varphi^1 = -\Delta\mathbf{L}\varphi^0 + \left(\lambda^0\Delta\mathbf{F}+\lambda^1\mathbf{F}\right)\varphi^0\\
&\vdots\\
&\left(\mathbf{L}-\lambda^0\mathbf{F}\right)\varphi^i = -\Delta\mathbf{L}\varphi^{i-1} + \sum_{j=0}^{i-1}\left(\lambda^{i-j-1}\Delta\mathbf{F}+\lambda^{i-j}\mathbf{F}\right)\varphi^j
\end{aligned}
\tag{5}
$$

The major drawback to this approach is that one needs to solve the recursive equations in Eq. (5) which are extremely time-consuming. Moreover, the recursive equations are dependent on the specific perturbation in the input parameters, i.e. $\Delta\mathbf{L}$ and $\Delta\mathbf{F}$. This means that Eq. (5) would have to be solved anew every time a perturbation is made to the system. This limits the GPT for the systems whose parameters have only small variations while first-order approximation is acceptable.

GPT can also be used to estimate the variations in any given response R:

$$
\begin{aligned}
\Delta R_{1st} &= \sum_{i=1}^{k}\frac{\partial R}{\partial \alpha_i}\Delta\alpha_i + \frac{\partial R}{\partial \phi}\Delta\phi\\
&= \sum_{i=1}^{k}\frac{\partial R}{\partial \alpha_i}\Delta\alpha_i - \left\langle \Gamma^*, \left(\Delta\mathbf{L}-\lambda\Delta\mathbf{F}\right)\phi\right\rangle
\end{aligned}
\tag{6}
$$

where the first term in Eq. (6) denotes as the direct effects which can be readily evaluated, and the generalized adjoint Γ^* is defined by the equation:

$$
\left(\mathbf{L}^*-\lambda\mathbf{F}^*\right)\Gamma^* = \frac{\partial R}{\partial \phi}, \text{ with } \left\langle \Gamma^*, \mathbf{F}\phi\right\rangle = 0 \tag{7}
$$

The Eq. (7) shows that the associated number of adjoint model executions of first-order GPT is dependent on the number of responses.

In the contrary, E$_P$GPT assumes that the flux variations lie in a small dimensional subspace, denoted hereinafter as active subspace, which are constructed by executing the forward model a number of times by employing range-finding algorithms [1, 2]. Moreover, the number of adjoint model executions is only dependent on the size of the active subspace.

As assumed, we can expand the flux variations in the active subspace as shown in the following equations:

$$
\Delta\phi = \sum_{i=1}^{r}\beta_i\mathbf{q}_i \tag{8}
$$

where r is the size of the active subspace, $\left\langle \mathbf{q}_i, \mathbf{q}_j\right\rangle = \delta_{ij}$ and $\beta_i = \left\langle \mathbf{q}_i, \Delta\phi\right\rangle$, for $i, j = 1, 2, \cdots, r$; δ_{ij} is the Kronecker symbol, and $\mathbf{q}_i$ represents an orthonormal basis vector function in the active subspace, which is only dependent on flux variations and can be determined by range-finding algorithms (RFA). RFA have been primarily developed in linear algebra community and the machine learning community [9]. The idea of RFA has been further extended by Abdel-Khalik and his research groups to identify a subspace in the input parameters space of complex engineering systems [1-2, 10]. Considering this is just a summary, we refer the reader to Ref. 9 for excellent review on the mathematical literature on range-finding algorithms.

After applying the E$_P$GPT manipulations, one can obtain the following equations for unknown coefficients:

$$
\boldsymbol{\beta} = -\left(\mathbf{I}+\mathbf{T}\right)^{-1}\mathbf{w} \tag{9}
$$

where $\left[\boldsymbol{\beta}\right]_i = \beta_i$, $\mathbf{I}\in\mathbb{R}^{r\times r}$ is identity matrix, and the elements in the matrix $\mathbf{T}\in\mathbb{R}^{r\times r}$ and vector $\mathbf{w}\in\mathbb{R}^{r}$ are given by:

$$
\left[\mathbf{T}\right]_{ij} = \left\langle \Psi_i^*, \Delta\mathbf{P}\mathbf{q}_j\right\rangle \text{ and } \left[\mathbf{w}\right]_i = \left\langle \Psi_i^*, \Delta\mathbf{P}\phi\right\rangle, \quad \text{for } i, j = 1, 2, \ldots, r
$$

and the generalized adjoint Ψ_i^* is the solution to the following equations:

$$
\mathbf{P}^*\Psi_i^* = \mathbf{q}_i - \left\langle \mathbf{q}_i, \phi\right\rangle, \text{ for } i = 1, 2, \cdots, r \tag{10}
$$

Furthermore, the exact variation in the eigenvalue could be approximated by:

$$
\Delta\lambda_{\text{E}_P\text{GPT}} = \frac{\left\langle \phi^*, \left(\Delta\mathbf{L}-\lambda\Delta\mathbf{F}\right)\phi\right\rangle + \boldsymbol{\eta}^T\boldsymbol{\beta}}{\left\langle \phi^*, \mathbf{F}\phi\right\rangle + \left\langle \phi^*, \Delta\mathbf{F}\phi\right\rangle} \tag{11}
$$

where $\left[\boldsymbol{\eta}\right]_i = \left\langle \phi^*, \Delta\mathbf{P}\mathbf{q}_i\right\rangle$, for $i = 1, 2, \cdots, r$.

It can be clearly seen from Eq. (10) that one needs to solve only r generalized adjoint equations to capture the exact variations in the flux and eigenvalue. Early works have shown that r is usually a small number compared to the original dimension of flux [10] in BWR assembly model.

CASE STUDY

The system considered for demonstration E$_P$GPT is a two-group infinite homogenous medium. For this case, the transport operators are 2 by 2 matrices such that one can easily obtain the analytic solution. The parameters for first group are arbitrarily assigned as $\Sigma_{t,1} = 5$, $\Sigma_{c,1} = 3$, $\Sigma_{f,1} = 1$, $\Sigma_{s,1\to1} = 0$, $\Sigma_{s,1\to2} = 1$, $\overline{\nu}_1 = 4$, and $\chi_1 = 0.75$ where the symbols have their usual definitions. Similarly,

the parameters for the second group are assigned as $\Sigma_{t,2}=2$, $\Sigma_{c,2}=1$, $\Sigma_{f,2}=1$, $\Sigma_{s,2\to1}=0$, $\Sigma_{s,2\to2}=0$, $\bar{\nu}_2=2$, and $\chi_2=0.25$. Notice that for each group the absorption $\left(\Sigma_c+\Sigma_f\right)_g\phi_g$ equals the neutron production $\left(\nu\Sigma_f\right)_g\phi_g$; therefore, the system is critical and the neutron transport operator can be obtained:

$$\mathbf{L}=\begin{pmatrix}\Sigma_{t,1}-\Sigma_{s,1\to1} & -\Sigma_{s,2\to1}\\ -\Sigma_{s,1\to2} & \Sigma_{t,2}-\Sigma_{s,2\to2}\end{pmatrix}=\begin{pmatrix}5 & 0\\ -1 & 2\end{pmatrix};$$

$$\mathbf{F}=\begin{pmatrix}\chi_1\nu_1\Sigma_{f,1} & \chi_1\nu_2\Sigma_{f,2}\\ \chi_2\nu_1\Sigma_{f,1} & \chi_2\nu_2\Sigma_{f,2}\end{pmatrix}=\begin{pmatrix}3 & 1.5\\ 1 & 0.5\end{pmatrix};$$

Moreover, $\mathbf{L}^*=\mathbf{L}^T$, and $\mathbf{F}^*=\mathbf{F}^T$. The characteristic equation for this problem is:

$$\begin{vmatrix}5-3\lambda & -1.5\lambda\\ -1-\lambda & 2-0.5\lambda\end{vmatrix}=0 \tag{12}$$

The fundamental forward solution is:

$$\lambda=1 \text{ and } \phi=\begin{pmatrix}\frac{3}{7} & \frac{4}{7}\end{pmatrix}^T$$

The fundamental adjoint solution is

$$\lambda=1;\ \text{and } \phi^*=\begin{pmatrix}0.5 & 0.5\end{pmatrix}^T$$

Note that all fluxes are normalized to one for simplicity. The perturbation equation for $\Delta\lambda$ is illustrated by considering the perturbation given by:

$$\Delta\mathbf{L}=\begin{pmatrix}\Delta\Sigma_{c,1} & 0\\ 0 & 0\end{pmatrix}$$

This perturbation represents a change in the capture cross section for the first group. The first order estimation for the variation in λ via GPT is:

$$\delta\lambda_{1st}=\frac{\left\langle\phi^*,\Delta\mathbf{L}\phi\right\rangle}{\left\langle\phi^*,\mathbf{F}\phi\right\rangle}=\frac{3}{20}\Delta\Sigma_{c,1} \tag{13}$$

The characteristic equation for the perturbed system can be solved to obtain the following exact result for the variation in λ resulting from the perturbation $\Delta\Sigma_{c,1}$:

$$\delta\lambda_{\text{Exact}}=\frac{3\Delta\Sigma_{c,1}}{20+\Delta\Sigma_{c,1}} \tag{14}$$

Considering the flux is normalized, only one basis vector is needed for EPGPT calculation since there is only one degree of freedom in the neutron flux variations. This basis vector is obtained by range-finding algorithm:

$$\mathbf{q}_1=\begin{bmatrix}1/\sqrt{2} & -1/\sqrt{2}\end{bmatrix}^T$$

A comparison of numerical results obtained using Eqs. (11), (13), and (14) are show in Table I and Table II.

Table I. Exact and Approximate Errors for $\Delta\lambda$

$\frac{\Delta\Sigma_{c,1}}{\Sigma_{c,1}}$	$\Delta\lambda_{\text{Exact}}$ (pcm)	ε_1 (pcm)	ε_2 (pcm)
0.01	449.33	-0.67	0.00
-0.01	-450.68	-0.68	0.00
0.05	2233.25	-16.75	0.00
-0.05	-2267.00	-17.00	0.00
0.10	4433.50	-66.50	0.00
-0.10	-4568.53	-68.53	0.00
0.25	10843.37	-406.63	0.00
-0.25	-11688.31	-438.31	0.00
0.50	20930.23	-1569.77	0.00
-0.50	-24324.32	-1824.32	0.00

where $\varepsilon_1=\Delta\lambda_{\text{Exact}}-\Delta\lambda_{1st}$; $\varepsilon_2=\Delta\lambda_{\text{Exact}}-\Delta\lambda_{\text{EpGPT}}$

Table II. Errors in Neutron Flux

$\frac{\Delta\Sigma_{c,1}}{\Sigma_{c,1}}$	rel.rms
0.01	1.43E-16
-0.01	2.63E-16
0.05	1.54E-16
-0.05	1.78E-16
0.10	1.67E-16
-0.10	1.97E-16
0.25	3.56E-16
-0.25	9.82E-17
0.50	1.44E-16
-0.50	1.64E-16

where $\text{rel.rms}=\frac{\left\|\phi_{\text{Exact}}-\phi_{\text{EpGPT}}\right\|_2}{\left\|\phi_{\text{Reference}}\right\|_2}$;

The fast group capture cross section is randomly perturbed by 10%. The results calculated by EPGPT and first-order GPT are compared to those computed by

solving the exact perturbed forward equation, as presented in Fig. 1 for 100 different cases.

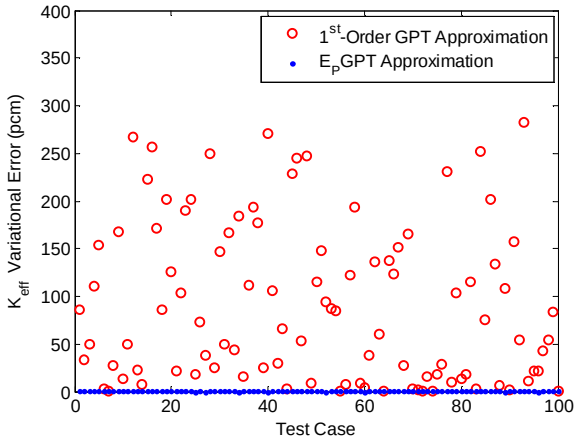

Fig. 1. Comparison of Estimation Accuracy (100 cases).

CONCLUSION

This presented summary has demonstrated that the solutions obtained by E_PGPT are equivalent to the solutions solved by the forward perturbed equations via a simple analytic example. However, by employing active subspace projection techniques, the E_PGPT places a high premium on reduction of the associated computational overhead required to estimate higher order variations.

We are currently working on employing E_PGPT to efficiently and accurately replace assembly calculations, currently used to prepare few-group cross sections for downstream core calculations.

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