EXACT-TO-PRECISION GENERALIZED PERTURBATION THEORY FOR NEUTRON TRANSPORT CALCULATION

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ABSTRACT

This manuscript extends the exact-to-precision generalized perturbation theory (E_pGPT), introduced previously, to neutron transport calculation whereby previous developments focused on neutron diffusion calculation only. The E_pGPT collectively denotes new developments in generalized perturbation theory (GPT) that place premium on computational efficiency and defendable accuracy in order to render GPT a standard analysis tool in routine design and safety reactor calculations. E_pGPT constructs a surrogate model with quantifiable accuracy that can replace the original neutron transport model for subsequent engineering analysis. This is achieved by reducing the effective dimensionality of the state variable (i.e. neutron angular flux) via projection onto an active subspace determined using reduced order modeling techniques. Confining the state variations to the active subspace allows one to recast the problem in terms of a small number of ‘pseudo’ responses which are solely dependent on the physics model rather than on the nominal number of responses, the input parameters, or the number of points in the state phase space. This renders a computationally efficient construction of the surrogate whose form is determined using a recursive relationship from the solution of the transport equation. Unlike conventional surrogate techniques, the E_pGPT can upper-bound the errors resulting from its predictions with high probability, which can be preset by the user.

Key Words: E_pGPT, GPT, Active Subspace, Pseudo Response

1. INTRODUCTION

In performing reactor analysis and design calculations, perturbation theory can significantly reduce the computational cost by bypassing the repeated execution of forward calculations, which is facilitated via adjoint calculations. Because of this property, GPT has found widespread use in many engineering-oriented applications such as sensitivity analysis, uncertainty quantification, and data assimilation, where one is interested in estimating a given response variation due to many input parameters perturbations (Baudron et al., 1998; Gandini, 2001; Geemert, 2001; Kim et al., 2001; Maldonado and Turinsky, 1995; Maldonado et al., 1995; Moore and Turinsky, 1998). Another example is the use of GPT for in-core fuel management optimization (Moore and Turinsky, 1998).

Perturbation theory was first introduced into reactor physics by Wigner (1945) for nonself-adjoint equations, and was subsequently further developed and customized, under the name of Generalized Perturbation Theory (GPT), for reactor analysis and design calculations (Gacuci et al., 1980; Gandini, 1967; Lewins, 1965; Oblow, 1976; Pomraning, 1965; Stacey, 1974; Usachev, 1964; Williams, 1986). Usachev (1964) developed the GPT, making exclusive use of importance

conservation concepts, for several physical processes taking place in a reactor working under steady-state conditions that are linear functionals of neutron flux. Gandini (1967) further extended the GPT to calculate the bilinear functionals of the real and adjoint fluxes, e.g. reactivity worth, reaction ratios.

It is noteworthy to mention that three most prominent GPT formalisms have been proposed by different scientists in 1960s and 1970s. The heuristic GPT developed by Usachev (1964) and Gandini (1967) associates the adjoint flux with concept of importance. Variational formalism developed by Lewins (1965), Pomraning (1965) and Stacey (1974) provides a sound theoretical basis for the GPT, and has found a much wider application in reactor physics approximations (Williams, 1986). The third formalism based on a formal differentiation of the response considered was proposed by Oblow (1978) and extensively developed by Cacuci et al. (1980). It is important to note that all the formalisms lead to identical variational expressions (Cacuci et al., 1980). In this work, the variational approach will be employed to develop the E_p GPT for neutron transport equation.

Currently, the first-order GPT has found its way into standardized computer codes that are available for routine reactor calculations; see for example the computer package SCALE 6.0 (Jessee et al., 2009). Employing first-order GPT, one can calculate the first-order derivatives for a given response with respect to all parameters using only one forward and one adjoint model executions (for the eigenvalue problem, the adjoint problem must be solved twice, once for the fundamental adjoint, and once for the generalized adjoint). Although very efficient, the accuracy is degraded when the parameters perturbations are outside the range that renders linear approximations acceptable.

With the introduction of the higher-order GPT, it has become possible to estimate the response variations to a very high level of accuracy (Baudron, 1998; Gandini, 1978; Greenspan and Gilai, 1978; McKinley and Rahnema, 2000; Mitani, 1973). Over the past four decades, the GPT theory has been rigorously extended to describe the higher-order derivatives of response. Unfortunately, as higher-order derivatives are sought, the computational cost becomes dependent either on the number of input parameters (Greenspan and Gilai, 1978) or the dimension of the space used to describe the forward solution (McKinley and Rahnema, 2000), i.e. the flux solution, depending on the higher-order GPT approach employed. These challenges have limited the use of GPT to linear models and investigative studies only.

Recently, we have introduced new developments into GPT, denoted by exact-to-precision GPT, or in short, E_p GPT, with initial application to neutron diffusion theory (Wang and Abdel-Khalik, 2012a, 2012b, 2011). The E_p GPT is based on a hybrid reduced order methodology that places a premium on computational efficiency to enable practical use in routine engineering calculations. E_p GPT combines both the forward and adjoint solutions to reduce the number of model executions required to calculate the variations of all model responses with respect to all model parameters taking into account all higher order of variations. In effect E_p GPT generates a surrogate model whose functional form is determined by the physics of radiation transport, and which can be used to replace the original transport model for the intended reactor application. Because of its reliance on a reduced order methodology, the surrogate constructed via E_p GPT can upper-bound its prediction errors when compared to the predictions of the original transport

model. This provides an enabling tool that can be used to analyze the impact of parameters variations on the responses variations for a wide range of applications such as generation of few-group constants for downstream core calculations, lattice design/optimization, fuel loading optimization, etc.

This manuscript discusses the theory of E_pGPT for transport models in Sec. 2, and demonstrates its use for representative reactor models in Sec 3. Sec. 4 provides some remarks about future work, and a recent implementation of the E_pGPT methodology under the SCALE6.2 BETA 2 version, in the form of a super-sequence, denoted by CRANE, which is intended for users to exercise the E_pGPT methodology for their applications.

2. E_pGPT MATHEMATIC DERIVATION

Let $\psi^*(\alpha)$ and $\psi(\alpha)$ both be functions of the same variables, represented by general symbol $\alpha \in \mathbb{R}^k$; the *inner product* of these two continuous functions is then expressed and defined by

$$\langle \psi^*, \psi \rangle = \int \psi^*(\alpha) \psi(\alpha) d\alpha \quad (1)$$

where the braces $\langle \rangle$ represent the integration that is carried over the whole accessible range of the variables. If $\psi^*(\alpha)$ and $\psi(\alpha)$ are any “well behaved” functions, in the sense that they satisfy certain boundary and continuity conditions, it is possible in the following way to define an operator $\mathbf{A}^*$ that is adjoint to $\mathbf{A}$:

$$\langle \psi^*, \mathbf{A}\psi \rangle = \langle \psi, \mathbf{A}^* \psi^* \rangle \quad (2)$$

Now consider the following time-independent form of the Boltzmann transport equation:

$$\mathbf{P}(\alpha)\phi = (\mathbf{L}(\alpha) - \lambda\mathbf{F}(\alpha))\phi = 0 \quad (3)$$

In this equation, the neutron angular flux, ϕ , is a function of continuous variables in space, energy, and direction and is determined by the input parameters as given by Eq. (3). The vector α of input parameters represents the input cross-section data, isotopic compositions, and geometry. The $\mathbf{P}$ operator represents all the terms in the transport equation, the $\mathbf{L}$ represents neutron loss terms only including leakage and absorption, and the $\mathbf{F}$ represents the fission process.

According to Eq. (2), the defining relationship for the neutron transport adjoint operator is:

$$\langle \phi^*, \mathbf{P}(\alpha)\phi \rangle = \langle \phi, \mathbf{P}(\alpha)^* \phi^* \rangle \quad (4)$$

where ϕ^* is the solution of

$$\mathbf{P}(\alpha)^* \phi^* = 0 \quad (5)$$

This equation is the adjoint transport equation and can be derived directly from the definition of the adjoint operator in Eq. (4) or from physical principles based upon importance. In addition, the boundary conditions for Eq. (5) are chosen to insure that Eq. (4) contains no boundary term contributions. The reference state with original value of input parameters α_0 of the system described in Eq. (3) will be denoted as

$$\mathbf{P}(\alpha_0)\phi_0 = 0 \quad (6)$$

or briefly denoted as:

$$\mathbf{P}_0\phi_0 = 0 \quad (7)$$

Similarly, the reference state for adjoint equation given in Eq. (5) can be written as

$$\mathbf{P}_0^*\phi_0^* = 0 \quad (8)$$

We will assume in the remainder of this discussion that there exists a numerical method that is used to solve Eqs. (7) and (8). Further we will assume that the numerical solution generates a discretized solution for the angular flux and its adjoint. Let n refers to the total number of components of the discretized angular flux. In this context, $\mathbb{N} = \mathbb{R}^n$ is denoted as the space in which the angular flux vector lives. The dual space is where the adjoint angular flux belongs.

Now consider an perturbed physical system, e.g. cross sections perturbations, control rod movements, described by

$$\mathbf{P}'\phi' = 0 \text{ or } \mathbf{L}'\phi' - \lambda'\mathbf{F}'\phi' = 0 \quad (9)$$

This system will be referred to as the perturbed state. The prime symbol will be used throughout this work to indicate a perturbed state. The convention used to relate the reference and perturbed states is illustrated by the following expression

$$\phi' = \phi_0 + \Delta\phi; \mathbf{P}' = \mathbf{P}_0 + \Delta\mathbf{P}; \mathbf{L}' = \mathbf{L}_0 + \Delta\mathbf{L}; \mathbf{F}' = \mathbf{F}_0 + \Delta\mathbf{F}; \lambda' = \lambda_0 + \Delta\lambda$$

where $\Delta\mathbf{P} = \Delta\mathbf{L} - \lambda_0\Delta\mathbf{F} - \Delta\lambda\mathbf{F}_0 - \Delta\lambda\Delta\mathbf{F}$ is referred to as the variation in operator $\mathbf{P}$, $\Delta\phi$ the angular flux variation, and $\Delta\lambda$ the change in the eigenvalue λ_0 . This convention will be maintained throughout this manuscript. To solve for the angular flux, a normalization condition is required, which is assumed to have the form:

$$\langle h, \phi \rangle = 1 \quad (10)$$

where h is typically selected to ensure that the power generated equals a user-defined value. We assume the normalization constant is 1.0.

The basic assumption of EpGPT is that one can expand the angular flux variations in a subspace $\mathbb{Z} \in \mathbb{N}$ with size r as shown in the following equations (the size of a subspace refers to the minimum number of independent vectors that can be used to describe any other vector that belong to the subspace):

$$\Delta\phi = \beta_1 q_1 + \beta_2 q_2 + \cdots + \beta_r q_r = \sum_{i=1}^r \beta_i q_i, \quad (11)$$

where, for convenience, we assume that the basis vectors are orthonormal such that:

$$\langle q_i, q_j \rangle = \delta_{ij}, \text{ and } \beta_i = \langle q_i, \Delta\phi \rangle, \text{ for } i, j = 1, 2, \dots, r;$$

δ_{ij} is the Kronecker symbol, and $\{q_i\}$ are the basis vectors that span the subspace $\mathbb{Z}$. This expansion assumes that any angular flux variation can be described as a linear combination of the basis vectors, wherein the coefficients $\{\beta_i\}$ are the only free variables that can change due to model parameters perturbations. This behavior has been observed in other scientific communities, see (Bui-Thanh et al., 2008; Chaturantabut and Sorensen, 2010; Halko et al., 2011) and the references within. The implication is that although the nominal model dimension is very high, very small sized subspace (denoted by the active subspace) can be used to approximate the dominant state (i.e., representing the angular flux in neutronics, temperature in thermal analysis, etc.) variations. If the active subspace is known or can be approximated with some level of confidence, the effective dimensionality of the model can be reduced resulting in significant computational savings.

The basic idea to construct the active subspace, as mentioned in (Wang and Abdel-Khalik, 2011), is by employing the range-finding algorithm which randomizes the execution of the forward model to produce snapshots, which are subsequently aggregated in a matrix and filtered using rank revealing decomposition techniques. The process is repeated until the subspace is large enough to meet a user-defined tolerance. In recent years, this algorithm has been rigorously proved by applied mathematicians; it has been shown that randomized operations could be used to approximate the range of matrix operators with high probability (Halko et al., 2011). More recent work has further developed this algorithm to bound the errors resulting from the restricting the flux variations to user-defined subspace (Abdo et al., 2015). In this paper, we will employ range-finding algorithm to reliably quantify the errors, and we recommend the readers to (Abdo et al., 2015; Halko et al., 2011) for the detailed description.

First, let us define the i^{th} pseudo response as:

$$R_i = \langle q_i, \phi \rangle, \text{ for } i = 1, \dots, r \quad (12)$$

The system equations, e.g. Eq. (3) and Eq. (10), are treated as constraint conditions upon the pseudo response. These constraints are then incorporated with the pseudo response using Lagrange multipliers to define an auxiliary functional as follows:

$$K_i[\alpha, \phi, \lambda, N_i^*, \Gamma_i^*] = R_i - N_i^* (\langle h, \phi \rangle - 1) - \langle \Gamma_i^*, \mathbf{P}(\alpha) \phi \rangle, \text{ for } i = 1, \dots, r \quad (13)$$

where Γ_i^* and N_i^* are the Lagrange multipliers associated with the two constraints in Eq. (3) and Eq. (10), respectively. Eq. (13) represents the basic idea behind the variational formalism proposed by Pomraning (1965). We need to stress that the functional K_i yields the exact result for the pseudo response R_i if the exact neutron angular flux ϕ and eigenvalue λ are used, which means that one can employ Eq. (13) instead of Eq. (12) to evaluate the variations in the pseudo response, e.g. $\Delta R_i = \Delta K_i$. Unlike the pseudo response expression in Eq. (12) which depends only implicit on the input parameters, the functional K_i depends explicitly on all the input parameters, as well as ϕ, λ, N_i^* and Γ_i^* . If one could make the auxiliary functional K_i stationary with respect to the variables λ and ϕ , i.e. the first-order variations of functional K_i with respect to the variables λ and ϕ are zero, then the variations in the K_i becomes only explicitly dependent on the input parameters perturbations. This is achieved as follows:

$$\left. \frac{\partial K_i}{\partial \phi} \right|_{(\alpha_0, \lambda_0)} = 0 \Rightarrow \mathbf{P}_0^* \Gamma_i^* = q_i - N_i^* h, \text{ for } i = 1, 2, \dots, r \quad (14)$$

$$\left. \frac{\partial K_i}{\partial \lambda} \right|_{(\alpha_0, \phi_0)} = 0 \Rightarrow \langle \Gamma_i^*, \mathbf{F}_0 \phi_0 \rangle = 0, \text{ for } i = 1, 2, \dots, r \quad (15)$$

The N_i^* are determined by requiring the RHS of Eq. (14) to be orthogonal to the reference forward angular flux:

$$\langle (q_i - N_i^* h), \phi_0 \rangle = 0 \Rightarrow N_i^* = \frac{\langle q_i, \phi_0 \rangle}{\langle h, \phi_0 \rangle}, \text{ for } i = 1, \dots, r \quad (16)$$

As one can observed from Eq. (14) and Eq. (16), Γ_i^* and N_i^* are independent of input parameters perturbations. Therefore, the first-order estimation for the variation in the pseudo response corresponding to the input parameters perturbations could be written as:

$$\Delta R_i|_{1st} = \Delta K_i|_{1st} = \frac{\partial K_i}{\partial \alpha} \Delta \alpha = - \left\langle \Gamma_i^*, \left(\frac{\partial \mathbf{P}}{\partial \alpha} \Delta \alpha \right) \phi_0 \right\rangle, \text{ for } i = 1, \dots, r \quad (17)$$

Unlike existing first-order GPT, E_pGPT determines the exact variation in the functional K_i due to variations in α , ϕ , and λ which is given by:

$$\begin{aligned}\Delta K_i &= \langle q_i, \Delta\phi \rangle - N_i^* \langle h, \Delta\phi \rangle - \langle \Gamma_i^*, (\mathbf{P}_0 \Delta\phi + \Delta\mathbf{P}\phi_0 + \Delta\mathbf{P}\Delta\phi) \rangle \\ &= \langle (q_i - N_i^* h - \mathbf{P}_0^* \Gamma_i^*), \Delta\phi \rangle - \langle \Gamma_i^*, \Delta\mathbf{P}\phi_0 \rangle - \langle \Gamma_i^*, \Delta\mathbf{P}\Delta\phi \rangle\end{aligned}\quad (18)$$

Note that the term $\langle \Gamma_i^*, \Delta\mathbf{P}\Delta\phi \rangle$ in Eq. (18) accounts for all higher-order terms that will appear in the variational expression for K_i . This term is neglected in the first-order GPT formulation, as indicated in Eq. (17). In the following derivation, we will show how to explicitly determine this term without having to resolve the perturbed system of equations.

First, EpGPT will set the first term in the RHS of Eq. (18) to zero for arbitrary change in ϕ , this could be as achieved by requiring

$$q_i - N_i^* h - \mathbf{P}_0^* \Gamma_i^* = 0 \quad (19)$$

Note that Eq. (19) is identical to the adjoint equation previously defined in Eq. (14), this is because the term $\langle (q_i - N_i^* h - \mathbf{P}_0^* \Gamma_i^*), \Delta\phi \rangle$ exactly represents the first-order variation of functional K_i with respect to the change in ϕ . In other words, the exact variation of functional K_i defined in Eq. (18) for EpGPT is stationary to changes in ϕ . And furthermore, N_i^* employed in Eq. (18) could be determined using the same expression defined in Eq. (16). The variation of functional K_i given in Eq. (18) reduces to

$$\Delta K_i = -\langle \Gamma_i^*, \Delta\mathbf{P}\phi_0 \rangle - \langle \Gamma_i^*, \Delta\mathbf{P}\Delta\phi \rangle, \text{ for } i = 1, \dots, r \quad (20)$$

Recall that $\Delta R_i = \Delta K_i$ and $\beta_i = \langle q_i, \Delta\phi \rangle = \Delta R_i$, one can rewrite Eq. (20) in a more compact form as follows:

$$\beta = -\varpi - \theta \quad (21)$$

where

$$\begin{aligned}\beta &= \begin{bmatrix} \beta_1 & \cdots & \beta_r \end{bmatrix}^T = \begin{bmatrix} \langle q_1, \Delta\phi \rangle & \cdots & \langle q_r, \Delta\phi \rangle \end{bmatrix}^T; \\ \varpi &= \begin{bmatrix} \langle \Gamma_1^*, \Delta\mathbf{P}\phi_0 \rangle & \cdots & \langle \Gamma_r^*, \Delta\mathbf{P}\phi_0 \rangle \end{bmatrix}^T; \theta = \begin{bmatrix} \langle \Gamma_1^*, \Delta\mathbf{P}\Delta\phi \rangle & \cdots & \langle \Gamma_r^*, \Delta\mathbf{P}\Delta\phi \rangle \end{bmatrix}^T\end{aligned}$$

Substitute Eq. (11) into $\Delta\mathbf{P}\Delta\phi$ yields:

$$\Delta\mathbf{P}\Delta\phi = \sum_{i=1}^r \beta_i \Delta\mathbf{P}q_i \quad (22)$$

Substituting Eq. (22) into the vector functional θ results in

$$\begin{aligned}
 \theta &= \left[\langle \Gamma_1^*, \Delta \mathbf{P} \Delta \phi \rangle \quad \cdots \quad \langle \Gamma_r^*, \Delta \mathbf{P} \Delta \phi \rangle \right]^T \\
 &= \left[\left\langle \Gamma_1^*, \Delta \mathbf{P} \left(\sum_{j=1}^r \beta_j q_j \right) \right\rangle \quad \cdots \quad \left\langle \Gamma_r^*, \Delta \mathbf{P} \left(\sum_{j=1}^r \beta_j q_j \right) \right\rangle \right]^T \\
 &= \left[\sum_{j=1}^r \beta_j \langle \Gamma_1^*, \Delta \mathbf{P} q_j \rangle \quad \cdots \quad \sum_{j=1}^r \beta_j \langle \Gamma_r^*, \Delta \mathbf{P} q_j \rangle \right]^T \\
 &= \begin{bmatrix} \langle \Gamma_1^*, \Delta \mathbf{P} q_1 \rangle & \cdots & \langle \Gamma_1^*, \Delta \mathbf{P} q_r \rangle \\ \vdots & \ddots & \vdots \\ \langle \Gamma_r^*, \Delta \mathbf{P} q_1 \rangle & \cdots & \langle \Gamma_r^*, \Delta \mathbf{P} q_r \rangle \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_r \end{bmatrix}
 \end{aligned} \tag{23}$$

Let's defining the following matrix functional

$$\mathbf{T} = \begin{bmatrix} \langle \Gamma_1^*, \Delta \mathbf{P} q_1 \rangle & \cdots & \langle \Gamma_1^*, \Delta \mathbf{P} q_j \rangle & \cdots & \langle \Gamma_1^*, \Delta \mathbf{P} q_r \rangle \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \langle \Gamma_i^*, \Delta \mathbf{P} q_1 \rangle & \cdots & \langle \Gamma_i^*, \Delta \mathbf{P} q_j \rangle & \cdots & \langle \Gamma_i^*, \Delta \mathbf{P} q_r \rangle \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \langle \Gamma_r^*, \Delta \mathbf{P} q_1 \rangle & \cdots & \langle \Gamma_r^*, \Delta \mathbf{P} q_j \rangle & \cdots & \langle \Gamma_r^*, \Delta \mathbf{P} q_r \rangle \end{bmatrix} \in \mathbb{R}^{r \times r}$$

Therefore, Eq. (23) could be rewritten as

$$\theta = \mathbf{T} \beta \tag{24}$$

Substituting Eq. (24) into Eq. (21) results in

$$\beta = -\varpi - \mathbf{T} \beta \tag{25}$$

Solving Eq. (25) for β , one can obtain

$$\beta = -(\mathbf{I} + \mathbf{T})^{-1} \varpi \tag{26}$$

where $\mathbf{I}$ is r by r identity matrix. Eq. (26) implies that one can calculate the exact coefficients using r adjoint model evaluations (i.e. Eq. (14)), all performed at the unperturbed state.

Therefore, the exact variation in the neutron angular flux of Eq. (11) can be approximated using the following equation:

$$\Delta\phi = \sum_{i=1}^r \beta_i q_i = \mathbf{Q}\beta = -\mathbf{Q}(\mathbf{I}_{r \times r} + \mathbf{T})^{-1} \varpi \quad (27)$$

Next, this approach enables one to estimate the exact variation in the eigenvalue. Multiplying Eq. (9) by ϕ^* and integrating yields

$$\langle \phi^*, \mathbf{P}'\phi \rangle = 0 \quad (28)$$

Eq. (28) can be solved for the exact variation in the eigenvalue to obtain

$$\Delta\lambda = \frac{\langle \phi_0^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F})\phi \rangle + \langle \phi_0^*, \Delta\mathbf{P}\Delta\phi \rangle}{\langle \phi_0^*, \mathbf{F}_0\phi_0 \rangle + \langle \phi_0^*, \Delta\mathbf{F}\phi_0 \rangle} \quad (29)$$

The second term in the numerator could be evaluated using Eqs. (22) and (26) to yield

$$\langle \phi_0^*, \Delta\mathbf{P}\Delta\phi \rangle = \sum_{i=1}^r \beta_i \langle \phi_0^*, \Delta\mathbf{P}q_i \rangle = \left[\langle \phi_0^*, \Delta\mathbf{P}q_1 \rangle \quad \cdots \quad \langle \phi_0^*, \Delta\mathbf{P}q_i \rangle \quad \cdots \quad \langle \phi_0^*, \Delta\mathbf{P}q_r \rangle \right] \beta$$

Let's define the following vector functional:

$$\eta = \left[\langle \phi_0^*, \Delta\mathbf{P}q_1 \rangle \quad \cdots \quad \langle \phi_0^*, \Delta\mathbf{P}q_i \rangle \quad \cdots \quad \langle \phi_0^*, \Delta\mathbf{P}q_r \rangle \right]^T$$

Eqs. (29) can be rewritten as

$$\Delta\lambda = \frac{\langle \phi_0^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F})\phi \rangle + \eta^T \beta}{\langle \phi_0^*, \mathbf{F}_0\phi_0 \rangle + \langle \phi_0^*, \Delta\mathbf{F}\phi_0 \rangle} \quad (30)$$

Since the $\Delta\mathbf{P}$ term depends on $\Delta\lambda$, we employ a Rayleigh quotient like iterative approach, originally proposed in Wang and Abdel-Khalik (2012a), to solve for $\Delta\lambda$. This approach is summarized as follows:

Rayleigh quotient like iterative approach to solve for $\Delta\lambda$:

- (a) Given $\Delta\lambda_k$, the k^{th} iterate for $\Delta\lambda$;
- (b) Calculate: $\Delta\mathbf{P}_k = \Delta\mathbf{L} - \lambda\Delta\mathbf{F} - \Delta\lambda_k\mathbf{F} - \Delta\lambda_k\Delta\mathbf{F}$;
- (c) Calculate: $\varpi, \mathbf{T}$ and η ;
- (d) Calculate: $\beta = -(\mathbf{I} + \mathbf{T})^{-1} \varpi$

(e) Calculate: $\eta^T \beta$

(f) Calculate the next iterate:
$$\Delta\lambda_{k+1} = \frac{\langle \phi_0^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F}) \phi_0 \rangle + \eta^T \beta}{\langle \phi_0^*, \mathbf{F}_0 \phi_0 \rangle + \langle \phi_0^*, \Delta\mathbf{F} \phi_0 \rangle}$$

(g) Continue until an appropriate stopping criterion is met

Once ϕ_0 , q_i , and Γ_i^* are obtained, the eigenvalue variations induced by input parameters perturbations can be estimated, with user-defined accuracy. In practice, this can be achieved as follows:

From pre-computation phase, one can obtain $\{q_i\}_{i=1}^r$ and $\{\Gamma_i^*\}_{i=1}^r$;

Given $\Delta\lambda_0=0$, $\Delta\lambda_1=10^{-5}$, $k=1$ and tolerance η ,

Calculate $A = \langle \phi_0^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F}) \phi_0 \rangle$, $B = \langle \phi_0^*, \mathbf{F}_0 \phi_0 \rangle + \langle \phi_0^*, \Delta\mathbf{F} \phi_0 \rangle$;

For $i, j = 1, \dots, r$

Calculate $[c_1]_i = \langle \phi_0^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F}) q_i \rangle$ and $[c_2]_i = \langle \phi_0^*, (\mathbf{F}_0 + \Delta\mathbf{F}) q_i \rangle$;

Calculate $[d_1]_i = \langle \Gamma_i^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F}) \phi_0 \rangle$ and $[d_2]_i = \langle \Gamma_i^*, \Delta\mathbf{F} \phi_0 \rangle$;

Calculate $[\mathbf{T}_1]_{i,j} = \langle \Gamma_i^*, (\Delta\mathbf{L} - \lambda_0 \Delta\mathbf{F}) q_j \rangle$ and $[\mathbf{T}_2]_{i,j} = \langle \Gamma_i^*, (\mathbf{F}_0 + \Delta\mathbf{F}) q_j \rangle$;

End

Do While $|\Delta\lambda_k - \Delta\lambda_{k-1}| > \eta$

Calculate the $r \times r$ parameter perturbation-induced matrix: $\mathbf{T} = \mathbf{T}_1 - \Delta\lambda_k \mathbf{T}_2$

Calculate $C_k = -(c_1 - \Delta\lambda_k c_2)^T (\mathbf{I}_{r \times r} + \mathbf{T})^{-1} (d_1 - \Delta\lambda_k d_2)$

Calculate the next iterate:
$$\Delta\lambda_{k+1} = \frac{A + C_k}{B}$$

$k = k + 1$

End While

Note that the EpGPT formulation only requires r adjoint model evaluations, all evaluated at the unperturbed state. Moreover, the higher order variations are all aggregated using an analytical expression. Finally, the accuracy of the EpGPT surrogate model depends on the active subspace selected for the flux. If no reduction is involved, the active subspace represents the entire state space, and the EpGPT estimates become exact. However due to restricting the flux to vary only over the active subspace, an error component is introduced. This component however can be estimated using rigorous error bounds that were introduced in previous work (Abdo, 2015). These features of EpGPT provide tremendous advantages over conventional higher order variational approach. First, because all the adjoint calculations required are done at the unperturbed state. Second, the user does not have to specify the order of variation required upfront, since the method aggregates all higher order of variations using analytical expression. Finally, the number of adjoint evaluations required is typically very small, and does not depend

on the nominal size of the state space nor the number of model parameters. This reduces the storage requirements, and renders the evaluation of the surrogate computationally inexpensive.

3. NUMERICAL RESULTS

In this manuscript, two cases based on the H.B. Robinson unit 2 PWR assembly BO-5 model (Radulescu et al., 2010) are employed to verify the usefulness and applicability of the E_pGPT theory. The modeling details for the first and second cases are provided in figure 1 showing the locations of burnable poison rods (BPR), e.g. borosilicate glass absorber rods, and neighboring fuel rods. The model is developed using a one-quarter assembly representation, taking advantage of the assembly symmetry. A reflective boundary condition was applied to the outer boundary of this configuration. The cross section data library v5-44 (or 44GROUPNDF5) is employed. Calculations are completed using SCALE 6.1 which is developed by ORNL. To implement the E_pGPT, the originally released SCALE 6.1 modules (e.g. NEWT and SAMS) are modified for the purpose of the experiments. Recently, the E_pGPT algorithm has been implemented directly inside SCALE as a new super-sequence called CRANE (Jessee and Dehart, 2011).

Figure 1. Model Layout with Grid Structure

Case I: Burnable poison rod insertion

The burnable poison rod (or BPR) insertion is achieved by increasing the poison material densities. Initial chemical composition and densities of BPR is provided in Table 1. The ranges of variations in the densities of BPR are shown in Table 2. For each perturbed case, all materials atom densities in BPR are perturbed as follows:

$$n_p = n_0 + \Delta n_{\max} \bullet \zeta \quad (31)$$

where vector n_p describes the perturbed atom densities, n_0 and $\Delta n_{\max}$ denotes the initial atom densities and maximum expected variations in the initial atom densities, respectively; ζ is a random value from the uniform distribution on the interval (0,1). Furthermore, the temperature variations in the fuel rod and moderator are achieved by randomly perturbing the microscopic cross-sections – fission, radiation capture, ν – by $\pm 10\%$. The dimension of the perturbed parameters space is $\alpha \in \mathbb{R}^{1107}$.

The eigenvalue at the reference condition for this case is given by $k_{\text{eff}} = 1.036746$, and the dimension of neutron angular flux space is $\phi \in \mathbb{R}^{1827936}$. The accuracy of E_pGPT approach is compared with direct forward approach. In this section, we use the ‘exact’ to represent the results predicted via the direct forward model execution of NEWT. For example, exact variations means the variations between the unperturbed reference solution and the perturbed solution predicted via the direct forward calculation.

Table 1. Atom Densities for BPR

Description	Material	Weight Percent	Atom Density (atoms/cm·barn)
BPR	o-16	53.53	4.1979E-02
	b-10	0.696	1.7941E-04
	b-11	3.186	3.6046E-03
	na-23	2.82	1.5369E-03
	al-27	1.758	8.1645E-04
	si	37.63	1.6791E-02
	k	0.33	1.0577E-04

Table 2. Atom Density Variations in BPR

Description	Material	Variations in Atom Density (atoms/cm·barn)
BPR	o-16	0.0 ~ 4.1979E-02
	b-10	0.0 ~ 1.7941E-04
	b-11	0.0 ~ 3.6046E-03
	na-23	0.0 ~ 1.5369E-03
	al-27	0.0 ~ 8.1645E-04
	si	0.0 ~ 1.6791E-02
	k	0.0 ~ 1.0577E-04

Figure 2 shows eigenvalue discrepancies between the direct forward calculation and the E_pGPT approximation against the size of the active subspace. For reference, the eigenvalue discrepancy between direct forward calculation and first-order GPT approximation is shown on the same graph as a horizontal line. As can be observed from figure 2, the first-order GPT predicts the eigenvalue variation in the wrong direction, while the E_pGPT can predict the eigenvalue variation within several *pcm*, compared to the direct forward prediction, using the active subspace with the size 55. Compared to size of the input space, the active subspace is pretty small.

Figure 2. Eigenvalue Tolerance versus r

And furthermore, we will calculate the response variations using the E_P GPT approach, where the response is defined as following:

$$R_g = \sum_{i=1}^{NOM} V_i \sum_{mm=1}^{NOA} \phi_{i,g,mm} w_{mm}, \text{ for } g = 1, \dots, NOG$$

For this case study, NOG is equal 44, thus we will evaluate 44 different responses using E_P GPT approach. In order to measure the accuracy of E_P GPT prediction, the results from the E_P GPT are compared with ‘exact variations’. For reference, figure 3 shows the 44 responses values at the reference condition versus the lethargy. The relative responses variations estimated by first-order E_P GPT, higher-order E_P GPT and direct forward approach (i.e. Exact Solution) are plotted in figure 4. As can be observed from figure 4, there is a big derivation in the predictions of response variations via the first-order E_P GPT and direct forward approach in the thermal energy range. Furthermore, there are three or four predictions in the responses via E_P GPT are less accurate than the rest predictions. If one examines the values of these responses in figure 3, one can find that these values are one or two orders of magnitude smaller than the rest of values. This phenomenon is usually caused by the approach used to construct the active subspace. The accuracy can be improved if one uses the relative or weighted angular flux to construct the active subspace.

Figure 3. Reference Response Values

Figure 4. Estimation of Response Variations (Relative and $r = 55$)

Moreover, the estimation accuracy is examined by using 30 test samples (i.e. $t = 30$). Figure 5 shows that the higher-order E_pGPT approach using 55 basis vectors can evaluate the k -

eigenvalue (or k_{eff}) variation much more accurately than the first-order GPT approximation; on the average the errors are reduced by two orders of magnitude. Figure 6 shows the *rms* error for all 30 test samples. Both figures 5 and 6 show that EpGPT can be employed to approximate the non-linear effects with high accuracy. The *rms* error is defined as following:

$$\text{Flux variation: } rms = \frac{1}{\sqrt{n}} \frac{\|\Delta\phi_{\text{exact}} - \Delta\phi_{\text{approx}}\|_2}{E(\phi)} \quad (32)$$

where the neutron angular flux $\phi \in \mathbb{R}^n$, $E(\phi)$ is the reference average neutron angular flux and Δ implies a variation from the reference calculations. The *rms* calculates the discrepancy between the exact variation estimated by direct neutron transport calculation and the variation estimated by EpGPT.

Figure 5. Comparison of Estimation Accuracy for Eigenvalue Variation ($t = 30$)

Figure 6. Analysis E_p GPT Errors for Angular Flux ($t = 30$)

Next, figure 7 compares the maximum errors for all 30 cases plotted in figure 6 to the error bound predicted by the range-finding algorithm (Wang and Abdel-Khalik, 2012a). Note that the error bound is consistently higher than the maximum angular flux variation error calculated between direct forward perturbations and E_p GPT approximation.

Figure 7. Angular Flux Variation Error vs. Size of Active Subspace

3.2 Design parameters perturbations

The H. B. Robinson Lattice BO-5 model is modified as follows:

Modification 1): each fuel pin is assigned with unique material identification number, and the different types of lattices are modeled only by perturbing material compositions and temperatures in the fuel pins;

Modification 2): The diagonally symmetric properties of the lattice are considered;

The modeling detail for the reference case is provided in Figure 8 showing the location of 31 unique fuel pins and the location of burnable position rod (the red circles). The original design characteristics are given in (Radulescu et al., 2010). The fuel density and temperature are chosen as the same as the original SCALE model, i.e. 9.550 g/cm^3 and 745 K. A reflective boundary condition was applied to the outer boundary of this configuration. In this model, the v5-44 cross section library is employed; S-6 quadrature, P-1 scattering (P-2 in the moderator), spatial and eigenvalue stopping criteria of $1.0\text{E-}5$ are used for NEWT forward calculations (Wang et al., 2015).

Figure 8. Model Layout and Grid Structure (Reference Case)

There're total 2274 computational cells for this lattice model. Thus, the dimension of neutron angular flux space is $2274 \times 44 \times 24 = 2401344$, i.e., $\phi \in \mathbb{R}^{2401344}$. The active subspace for this study is constructed from the random perturbations of fuel rod densities, temperatures and enrichments. The fuel rod density is randomly selected from 9.0725 g/cm^3 to 10.0275 g/cm^3 , as well as the fuel rod temperature is randomly selected from 600 K to 1100 K for each unique fuel pin. The fuel temperature range at different operating condition is from 676.75 K to 1041.27 K (Radulescu et al., 2010). The temperature perturbation range for this study is chosen larger than the one in (Radulescu et al., 2010) in order to build an active subspace that can capture response variations due to all possible temperature perturbations. In (Radulescu et al., 2010), there are three different types of fuel enrichments, i.e. region 1: 1.85 wt%, region 2: 2.55 wt%, and region 3: 3.10 wt%. The maximum fuel enrichment and minimum fuel enrichment for this study are

chosen 20% higher than region 3 and 20% lower than region 1. In other words, the fuel rod enrichment is randomly selected from 1.48 wt% to 3.72 wt%. Two cases with different enrichments at three different operating temperatures are employed here to examine the capability of EpGPT for lattice design calculations. Table 3 shows the discrepancies in eigenvalue predictions between the EpGPT and the direct neutron transport calculation. For comparison, the discrepancies in eigenvalue predictions between the first-order GPT and the direct neutron transport calculation are also presented in table 3. As can be observed from table 3, the maximum variation in the eigenvalue is -11743 pcm (case II-c), while the maximum discrepancy in the eigenvalue prediction is only 39.8 pcm (case II-b).

Table 3. Discrepancy in the Eigenvalue Prediction

	case I-a	case I-b	case I-c	case II-a	case II-b	case II-c
Enrichment	U-235: 3.10 wt %			U-235: 1.85 wt %		
Temperature (K)	743	675	1000	743	675	1000
Nominal Case	$k_0 = 1.037250$					
k'	1.098615	1.101001	1.092005	0.925610	0.927727	0.919813
$k' - k_0$ (pcm)	6136.5	6375.9	5475.5	-11164.1	-10952.3	-11743
$k' - k_{1st}$ (pcm)	-820.8	-806.5	-861.4	-1942.2	-1960.2	-1892.1
$k' - k_{EpGPT}$ (pcm)*	-6.6	-2.3	-19.5	39.1	39.8	31.0

* The size of active subspace employed for EpGPT calculation in this table is 20.

Figure 9 plots the *rms* errors in angular flux variations against the size of active subspace. As the size of active subspace is increased, the associated errors in the angular flux variations are reduced accordingly since the active subspace starts to capture a larger component of angular flux variations. Analysis of figure 9 indicates that first-order approach is not accurate enough for the large variations in the fuel enrichments. In addition, the first-order EpGPT approach is equivalent to the first-order GPT approach in *rms* metric, which has been demonstrated in (Wang, 2013).

Figure 9. Analysis of E_pGPT Errors versus the Size of Active Subspace

4. CONCLUSIONS

Our new developments in generalized perturbation theory, referred to as E_pGPT have been demonstrated previously for diffusion theory calculations and now transport theory calculations. E_pGPT's overarching goal is to realize the power of GPT in realistic reactor calculations where nonlinear effects are important, and when conventional GPT approach is computationally intractable. E_pGPT achieves computational efficiency by noticing that the angular flux variations, despite their high dimensionality, can be well-approximated by an active subspace of very small size as compared to the nominal angular flux space dimension. By projecting all the angular flux equations and the associated responses onto the active subspace, one can reduce the associated computational overhead required to estimate higher-order variations using GPT. Because of its reliance on reduced order modeling to capture the active subspace, E_pGPT can provide a reliable estimate on the errors resulting from its predictions, where is not possible with conventional GPT theory. This study has examined the performance of E_pGPT for cross sections, fuel density, enrichment and temperature perturbations.

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