



Exact-to-precision generalized perturbation theory for neutron transport calculation



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HIGHLIGHTS

- We extend the exact-to-generalized perturbation theory to neutron transport calculations.
- E_pGPT can upper-bound the errors resulting its predictions with high probability.
- We have applied E_pGPT to lattice physics calculations.

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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.

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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; Van 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 (Cacuci 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.

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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 [Oblov \(1976\)](#) 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 EpGPT 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, EpGPT, with initial application to neutron diffusion theory ([Wang and Abdel-Khalik, 2012a, 2012b, 2011](#)). The EpGPT is based on a hybrid reduced order methodology that places a premium on computational efficiency to enable practical use in routine engineering calculations. EpGPT 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 EpGPT 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 EpGPT 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 EpGPT for transport models in Section 2, and demonstrates its use for representative reactor models in Section 3. Section 4 provides some remarks about future work, and a recent implementation of the EpGPT 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 EpGPT methodology for their applications.

2. EpGPT 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 a perturbed physical system, e.g. cross sections perturbations, control rod movements, described by

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

This system will be referred to as the perturbed state. The prime symbol will be used throughout this work to indicate a perturbed

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