Further GPT-free Developments for Monte Carlo Models

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INTRODUCTION

The GPT[1]-free method has been recently introduced to eliminate the need to solve the inhomogeneous eigenvalue problem required to perform GPT-based sensitivity analysis [1-2]. The solution of this equation is often difficult with slower convergence than the homogeneous eigenvalue problem. The GPT-free method employs a reduced order model (ROM) based on subspace theory to explore for sensitivity information of generalized responses using only the solution of the homogeneous adjoint eigenvalue problem. In the standard perturbation theory, this adjoint solution is often referred to as the fundamental adjoint flux which is used in conjunction with the forward flux to determine the sensitivities of the eigenvalue with respect to cross-sections. Given that only the homogeneous eigenvalue problem is needed to find responses sensitivities, the use of GPT-free method can be shown to be advantageous over standard GPT method for models with many responses, where in standard GPT method, a separate adjoint solution is required for each response of interest. Moreover, the use of GPT-free method is also advantageous for models where the construction of the GPT equations is infeasible or impractical.

It is noteworthy to mention that GPT developments have been mainly confined to deterministic models with very little effort to extend the theory to Monte Carlo (MC) models. With the exception of the fundamental adjoint that can be calculated in MC codes, there is no clear way for implementing GPT into existing Monte Carlo codes such as MCNP [3] or KENO [4]. The GPT-free methodology is particularly advantageous for such situation since the standard GPT formulation is not required.

The idea of GPT-free method is based on the fact that the eigenvalue of a reactor system is implicitly dependent on all generalized responses, which are both functions of the flux [1-2]. This implies that the sensitivities of generalized responses with respect to nuclides cross-sections can be represented as a linear combination of eigenvalue sensitivities. The GPT-free method employs this idea to identify a subspace in the input parameters (often representing cross-sections) space, with dimension r much smaller than the number of input parameters n. If r is sufficiently small, one can employ a forward sensitivity analysis in search for sensitivity information. In previous work, this approach was demonstrated successfully. In this summary, we introduce a new development to further reduce the computational cost associated with the forward sensitivity analysis required.

For typical reactor models with sufficient details, the cross-sections can number in the hundreds of thousands and more, while the dimension of the reduced subspace is found to be in the order of several hundreds. The implication is that several hundred forward runs are required to generate the sensitivities of all responses with respect to all cross-sections. Although this is a huge reduction in the computational overhead, we believe several hundred executions could still be considered prohibitive, especially by end-users and practitioners like industry personnel and regulators. We show in this summary that this cost could be reduced by another order of magnitude, which should prove useful for routine calculations.

BACKGROUND OF PROPOSED APPROACH

To illustrate the idea behind the proposed approach, we consider a MC model with a given cross-section that is assumed uncertain. Assuming one has a reliable approach to propagate this uncertainty, the response uncertainty will be impacted by two sources of uncertainties, uncertainty due to the input cross-section uncertainty, and the statistical uncertainty resulting from the stochastic simulation. The former is often referred to as epistemic uncertainty, while the latter is aleatoric uncertainty.

Aleatoric uncertainty results from the randomness inherent in the physical phenomenon being simulated, e.g. radiation transport and interaction with the medium, while epistemic uncertainty originates from lack of knowledge due to inadequacies in the experimental procedure or lack of complete measurements [5]. Aleatoric uncertainties of the responses can be reduced by increasing the number of MC particle history, while epistemic uncertainties can be reduced using a data assimilation approach with low uncertainty measurements.

The GPT-free method currently relies on a forward sensitivity analysis to calculate responses variations. This requires one to ensure the epistemic and aleatoric uncertainties are well-resolved. To ensure that, each simulation is executed with enough number of particles to

[1] GPT stands for Generalized Perturbation Theory

ensure the aleatoric uncertainty is orders of magnitude less than the expected epistemic uncertainties.

Given however the independence of aleatoric and epistemic uncertainties for neutronics calculations, and given that one is interested in first order variations only, the responses aleatoric and epistemic uncertainties are expected to be independent as well. A recent study has confirmed this hypothesis by showing that one could reliably separate the contribution of aleatoric and epistemic uncertainties with substantially reduced computational efforts realized by using one or two orders of magnitude particle histories in MC simulation [5].

IMPLEMENTATION OF PROPOSED APPROACH

The GPT-free method is modified from its standard form shown in Ref [1-2] as follows:

1. Perform reference MC simulation with enough number of particle histories to reach the desired level of statistical uncertainties.
2. Perform *r* (r is the estimated rank) MC simulations using a much smaller number of particle histories used in step 1, wherein each simulation the cross-sections are randomly perturbed in a statistically consistent manner within their prior uncertainties. Reduce both the convergence tolerance limit and the total number of MC histories by one order of magnitude each. These simulations generate the sensitivities of the eigenvalue with respect to the cross-sections. Note, in KENO [4], this is equivalent to performing *r* forward and *r* adjoint simulations, whereas in MCNP, the sensitivities of the eigenvalue are calculated directly without explicit formulation of the adjoint flux [6].
3. Identify the sensitivity subspace in a similar manner to the current GPT-free algorithm, and determine effective rank of the subspace via a rank finding algorithm.
4. Perform forward sensitivity analysis based on the subspace and effect rank obtained from step 3 and 4
5. End

RESULTS FOR AN ASSEMBLY PROBLEM

These new development for GPT-free method was tested in the same assembly model problem as depicted in previous work [2]. The BWR assembly consists of 91 fuel pins laid over 10 x 10 grid with a square-shaped coolant channel in the middle. The average fission spectrum, the fission and capture cross-sections of 9 fuel nuclides (^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu) and the capture cross-sections of 14 notable fission products (^{131}Xe, ^{135}Xe, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{152}Gd, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{160}Gd) are considered as input parameters in this study. Take into account of 238 energy groups and 7 different fuel mixtures, the total number of input parameters is readily calculated as: (3 x 9+14) x 238 x 7 = 68306.

The eigenvalue in the reference calculation is given by: $k = 1.0723 \pm 0.0001$, where the statistical uncertainty of the eigevalue is maintained to be the order of 10 PCM. This error represents deviations in *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.

The sensitivities of the eigenvalue with respect to these parameters, which are necessaries for GPT-free method, were calculated by TSUNAMI-3D [6] sequence in SCALE-6.0 package [7]. And GPT-free method usually utilizes hundreds of sensitivity profiles by randomly sampling the nuclide cross sections in order to fully capture the sensitivity subspace of the general response [1]. In other words, the TSUNAMI sequence, which includes one forward and one adjoint Monte Carlo calculation, are enforced to be executed for hundreds of times. Numerical experience shows the computation time of one TSUNAMI sequence for this simple assembly model with one single 3.0GHz CPU is about 3-4 hours. As aforementioned analysis pointed out, a reduced order model can be investigated here to alleviate the computational headache aroused from the procedure of identifying the efficient sensitivity subspace. In the test problem, the computational overhead at this point is reduced by manually releasing some key control parameters of the program. For example, the criterion of iterative convergence to eigenvalue and the simulated Monte-Carlo particles per iterative cycle are both lessened by a factor of 10 in contrast to the ones configured in the reference calculation. Experience shows the single TSUNAMI sequence can be finished within 10 minutes with the loose parameters, which indicates that significant computational efforts can be saved if considering hundreds or thousands of sequences are required to execute in GPT-free method.

Certainly, with loosed convergence tolerance limit, the statistical (aleatoric) uncertainty of each individual response is consequently increased, however, since the aleatoric error is independent of epistemic one, the uncertainties of the sensitivity subspace (which mainly caused by epistemic factors) stays unchanged. The results demonstrated from the test problem verify this presumption.

Fig.1 illustrates the validation of the efficient subspace via *k* eigenvalue response. The reference eigenvalue is depicted as a solid red line with the value of 1.0723. The eigenvalues of 30 other cases with cross sections randomly perturbed are depicted with black circle line. Since the group-wised cross sections in these 30 perturbed cases are randomly perturbed with -25% to 25% from reference ones in the study, the eigenvalues of the 30 cases fluctuates around the reference eigenvalue as demonstrated in Fig. 1.

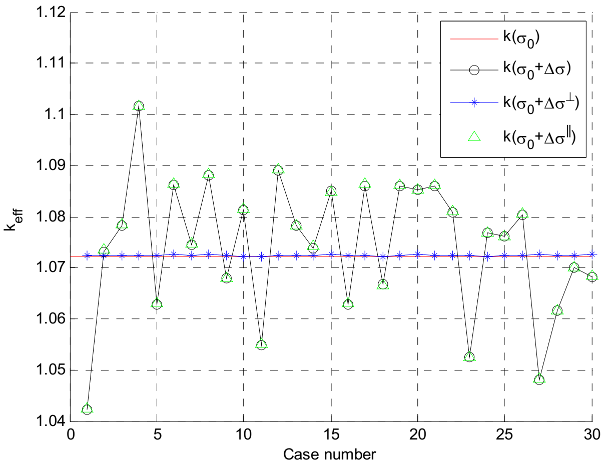

Fig. 1. Verification of efficient subspace via k eigenvalue response

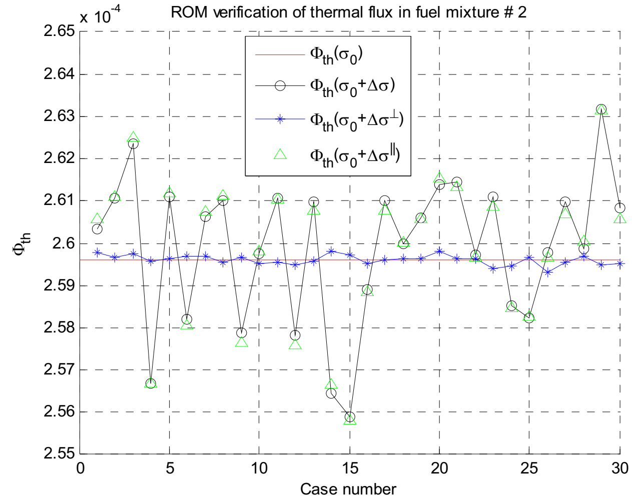

Fig. 2. Verification of efficient subspace via thermal flux.

The blue line and the triangular green dots in Fig. 1 represent two approximated eigenvalue for the perturbed cases. Here $\Delta\sigma^{\perp} = \left(I - \mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\sigma$ and $\Delta\sigma^{\parallel} = \left(\mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\sigma$ are respectively orthogonal and parallel component of $\Delta\sigma$ as it projects onto the subspace $\mathbf{Q}_r$, while $\mathbf{Q}_r$ (r = 619) is the efficient sensitivity subspace constructed from reduced GPT-free method. The behavior of the curves in Fig. 1 basically proves the following identities:

$$\begin{aligned} k(\sigma_0 + \Delta\sigma^{\perp}) &= k(\sigma_0) \\ k(\sigma_0 + \Delta\sigma^{\parallel}) &= k(\sigma_0 + \Delta\sigma) \end{aligned}, \qquad (1)$$

which on the other side implies $\mathbf{Q}_r$ fully captures the effect of sensitivity subspace, because if $\mathbf{Q}_r$ did not accurately approximate the sensitivity subspace, the identities in Eq. (1) cannot be perfectly hold.

Additional verification study is also carried out via thermal flux response. The results are illustrated in Fig. 2. Without loss of generality, the verification in Fig. 2 only utilizes the thermal flux response of fuel mixture # 6 (with 2.82% U-235 enrichment). The behavior of the curves in Fig. 2 conveys the same information as the one rendered in Fig. 1, which is the sensitivity subspace the response is successfully and accurately constructed with much greatly reduced GPT-free method.

CONCLUSIONS

The new development of constructing sensitivity subspace for GPT-free method in Monte Carlo models is described and successfully tested in a problem of realistic BWR assembly model calculations. The sensitivity subspace of generalized response with respect to cross sections in Monte Carlo models can be constructed with significantly reduced effort comparing to common treatments in this regard, and the efficiency of the subspace is preserved via the verification process of various responses.

Ongoing endeavor for this project is to extend this methodology to include depletion functions in reactor analysis and also pursue success of reducing computation overheads when applying the GPT-free method to other Monte Carlo modeling systems.

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