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Application of GPT-Free Method to Sensitivity Analysis in Monte Carlo Models

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Introduction

- **Sensitivity Analysis (SA)** determines the significance of the contribution of input parameters for the output responses, meanwhile it provides complementary values to **Uncertainty Quantification (UQ)** procedure.
- **Forward Sensitivity Analysis (FSA)** is efficient if the number of responses of interest in the problem considerably exceeds the number of parameters, while **Adjoint Sensitivity Analysis (ASA)** is advantageous for systems with a large number of parameters.
- **Deterministic** Models are superior when performing SA because they can be intrusively modified, and the cost is low, whereas SA for **Monte Carlo** model is difficult because of the ASA formulation is not straightforward (to our knowledge, never been done before), and requires unaffordable computational overheads.

Generalized Perturbation Theory (GPT)

- The adjoint formulation in traditional perturbation theory (PT) enables one to efficiently predict the change in eigenvalue k due to perturbed cross-sections in reactor analysis.
- GPT expands PT to determine variations of generalized responses, e.g. bilinear ratios of responses.
- Both PT and GPT provide an efficient tool to calculate sensitivities in various applications.

Perturbation Theory	Generalized Perturbation Theory
Eq: $\left(\mathbf{L}^* - \frac{1}{k}\mathbf{F}^*\right)\phi^* = 0$	**Eq:** $\left(\mathbf{L}^* - \frac{1}{k}\mathbf{F}^*\right)\Gamma^* = \frac{dR}{d\phi}$
Sensitivity: $\frac{dk}{d\sigma}$	**Sensitivity:** $\frac{dR}{d\sigma}$

Limitations of GPT

- In applications where both the number of input parameters and output responses are significantly large, GPT can become computationally intractable due to the considerable number of adjoint calculations needed.
- For those engineering systems that are modeled stochastically, e.g., the Monte Carlo particle transport model commonly used in reactor analysis benchmark calculations, there currently exists no general extension of GPT theory.

We are thereby motivated to develop GPT-free method.

GPT-Free: Overview

- Objectives of GPT-free method:
  - Generate sensitivity profiles of generalized responses of interest with respect to input parameters **without formation or solution** of the GPT-based adjoint equations.
  - **Reduce computational overhead** in computing response sensitivity profiles for high dimensional models with many inputs and outputs.

- GPT-free method constructs a reduced order model (ROM) to efficiently complete sensitivity analysis (SA) by using the fundamental homogenous adjoint based on perturbation theory (PT).

- Response sensitivities can then be used for nuclear calculations such as Uncertainty Quantification and Design Optimization.

GPT-Free: Theory

1. The system multiplication, k, can be written as an unknown function of the state-space (neutron flux), ϕ

$$k = f\left(\phi\right)$$

2. Consider a response functional that is an inner product of some cross-sections, σ, and the flux

$$R = \left\langle \phi, \sigma \right\rangle$$

3. The multiplication may be implicitly related to all generalized responses of interest, described mathematically as:

$$k = f\left(R_1 \ldots R_m\right)$$

4. Differentiate with respect to cross-sections

Fundamental Sensitivity Profile

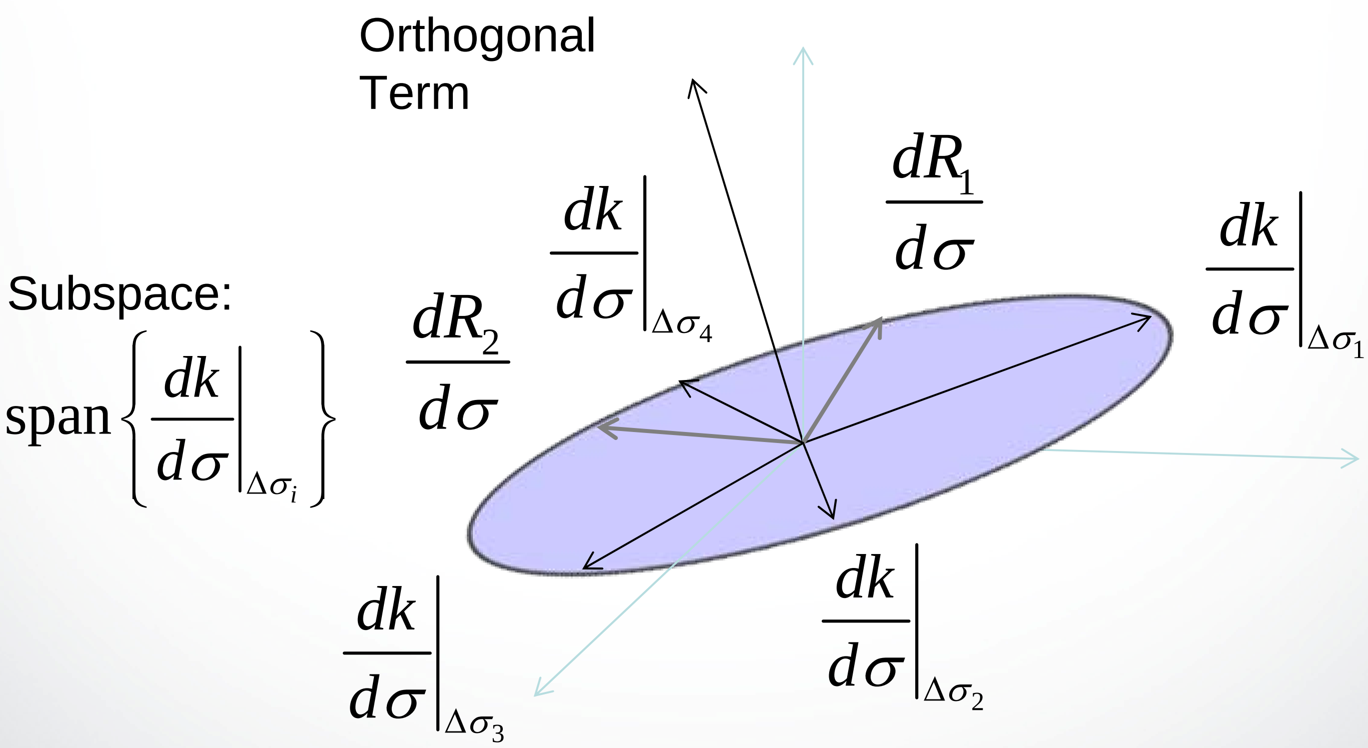
$$\boxed{\frac{dk}{d\sigma}} = \sum_{i=1}^{m} \frac{\partial f}{\partial R_i} \boxed{\frac{dR_i}{d\sigma}}$$

General Response Sensitivity Profiles

Constructing Equivalent Subspace

Cross sections are randomly sampled in order to construct the equivalent subspace spanned by the sensitivity vectors.

$$\frac{dk}{d\sigma} = \sum_{i=1}^{m} \frac{\partial f}{\partial R_i} \frac{dR_i}{d\sigma}$$

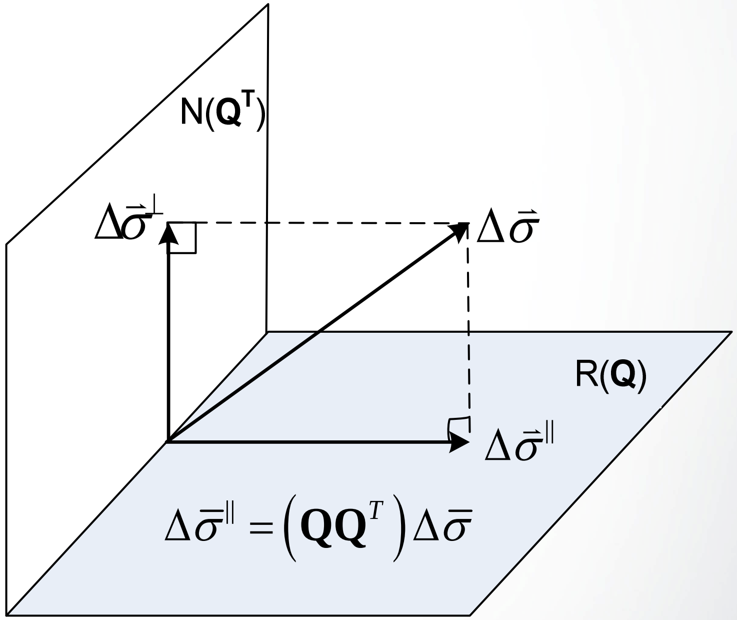


Project Parameter Perturbation onto Sensitivity Subspace

Let $\mathbb{N}$ denote the subspace determined by the GPT-free method, and Let $\mathbf{Q}_r$ be an orthonormal matrix of rank r whose columns span the subspace $\mathbb{N}$. The parameter perturbation may be decomposed into two orthogonal components: $\Delta\vec{\sigma} = \Delta\vec{\sigma}^{\parallel} + \Delta\vec{\sigma}^{\perp}$

Where: $\Delta\vec{\sigma}^{\parallel} = \left(\mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\vec{\sigma}$

$$\Delta\sigma^{\perp} = \left(\mathbf{I} - \mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\vec{\sigma}$$



$$f\left(\vec{\sigma}_0 + \Delta\vec{\sigma}\right) = f\left(\vec{\sigma}_0 + \Delta\vec{\sigma}^{\parallel}\right) \text{ !!!}$$

Reduced Order Modeling (ROM) Technique for Forward Based SA

- The key step in forward **SA** is to perform calculation: $f\left(\vec{\sigma}_0+\Delta\vec{\sigma}\right)$
- **Regular approach** assumes: $\Delta\vec{\sigma}=\sum_{i=1}^{n}\Delta\sigma_i\mathbf{e}_i$

  Then,

$$f\left(\vec{\sigma}_0+\Delta\vec{\sigma}\right)=f\left(\vec{\sigma}_0+\sum_{i=1}^{n}\Delta\sigma_i\mathbf{e}_i\right)\overset{\text{if linear}}{=}f\left(\vec{\sigma}_0\right)+\sum_{i=1}^{n}\Delta\sigma_i\left[f\left(\vec{\sigma}_0+\mathbf{e}_i\right)-f\left(\vec{\sigma}_0\right)\right]$$

  This procedure requires ***n*** forward executions.

- **ROM approach** assumes: $\Delta\vec{\sigma}^{\parallel}=\left(\mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\vec{\sigma}=\sum_{i=1}^{r}\vec{q}_i\left(\vec{q}_i^T\Delta\vec{\sigma}\right)=\sum_{i=1}^{r}\alpha_i\vec{q}_i$

  Then, $f\left(\vec{\sigma}_0+\Delta\vec{\sigma}\right)\approx f\left(\vec{\sigma}_0+\Delta\vec{\sigma}^{\parallel}\right)$

$$=f\left(\vec{\sigma}_0+\sum_{i=1}^{r}\alpha_i\vec{q}_i\right)\overset{\text{if linear}}{=}f\left(\vec{\sigma}_0\right)+\sum_{i=1}^{r}\alpha_i\left[f\left(\vec{\sigma}_0+\vec{q}_i\right)-f\left(\vec{\sigma}_0\right)\right]$$

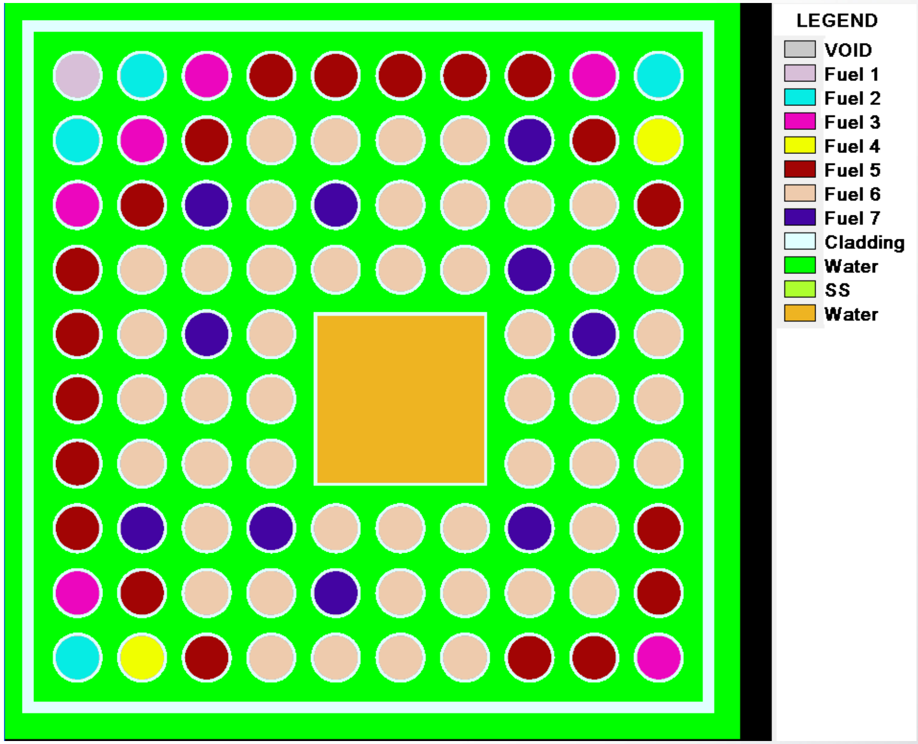
This procedure requires only ***r*** forward executions.

r << n !!!

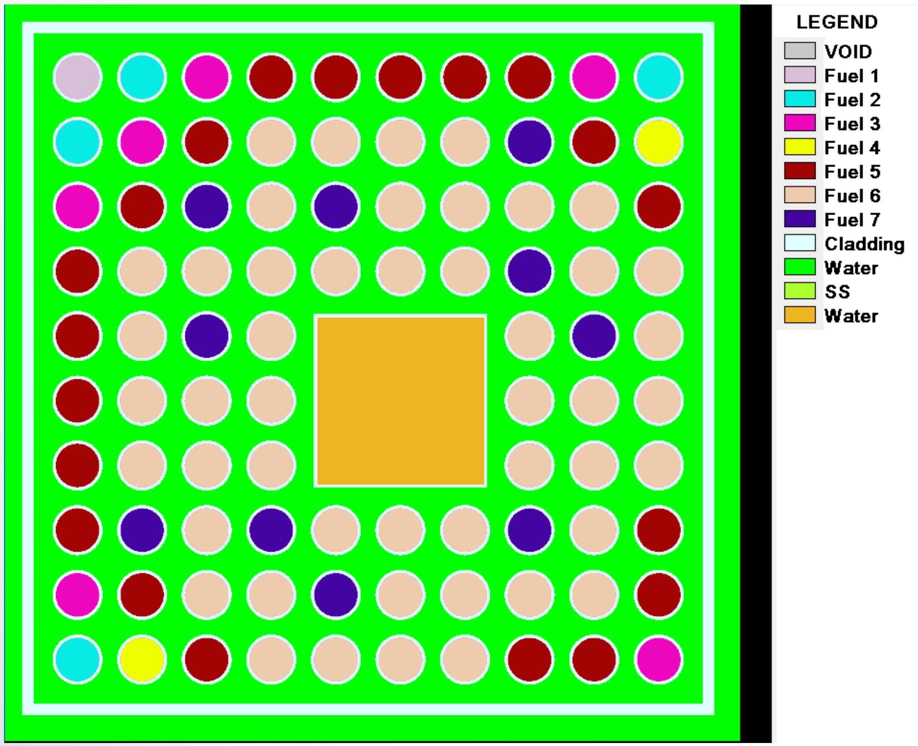
Numerical Applications

Case Study: BWR Assembly Model

- Code: *TSUNAMI-3D* sequences in *SCALE* package
- BWR Assembly: 91 fuel pins laid over 10x10 grid with a coolant channel in the middle and fuel pins designed with 7 different U-235 enrichments
- Criticality calculation
- Monte Carlo based particle transport solver (*KENO-V.a*)



High Dimensionality Problem



Isotopes: **20**
Reactions: **3**
Energy Groups: **238**
Fuel Regions: **7**

Number of Input parameters:

$$n = 68306$$

Reference eigenvalue:

$$k = 1.0723 \pm 0.0001$$

Range *r* Finding Algorithm (κ-Metric)

- Randomly perturb cross sections $\bar{\sigma}_{\text{pert},i} = \bar{\sigma}_0 + \Delta\bar{\sigma}_i$
- Execute the sensitivity analysis sequence in SCALE to calculate $\left. dk/d\bar{\sigma} \right|_i$
- Repeat *r* times and form the decomposition:

$$\mathbf{QR} = \left[\left. dk/d\bar{\sigma} \right|_1 \quad \ldots \quad \left. dk/d\bar{\sigma} \right|_r \right] \in \mathbb{R}^{n \times r}$$

- Evaluate the κ-metric; increase ***r*** until the error of the metric is below user-defined tolerance

The specific form of κ-metric is application-dependent.

The κ-Metric for Eigenvalue

The κ-metric is defined as:

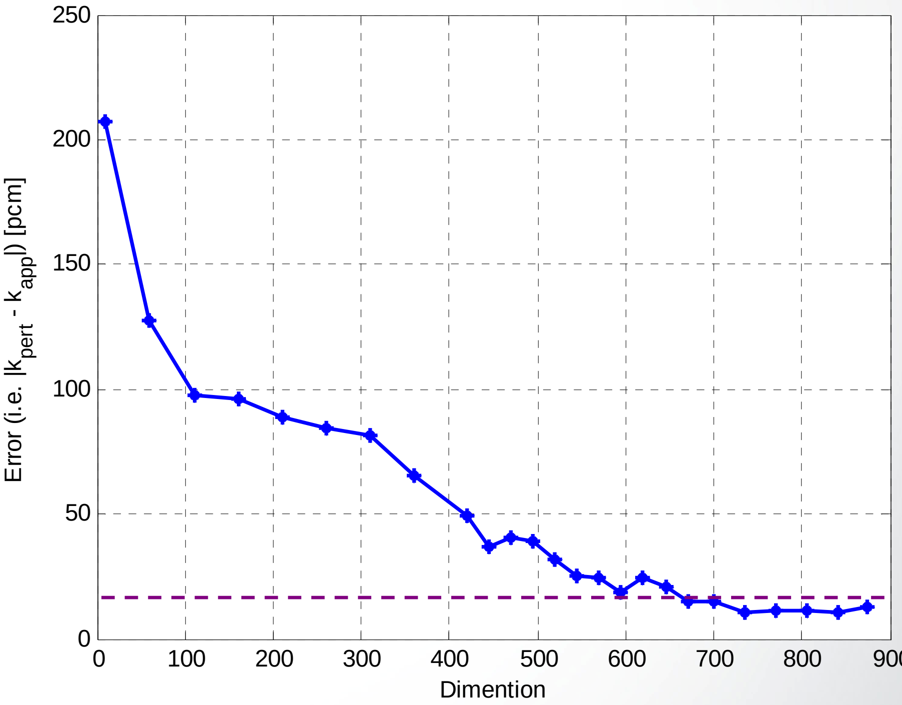
$$\kappa = \left| k_{\text{pert}} - k_{\text{app}} \right|$$

Where,

$$k_{\text{pert}} = k\left(\vec{\sigma}_0 + \Delta\vec{\sigma}\right)$$

$$k_{\text{app}} = k\left(\vec{\sigma}_0 + \Delta\vec{\sigma}^{||}\right)$$

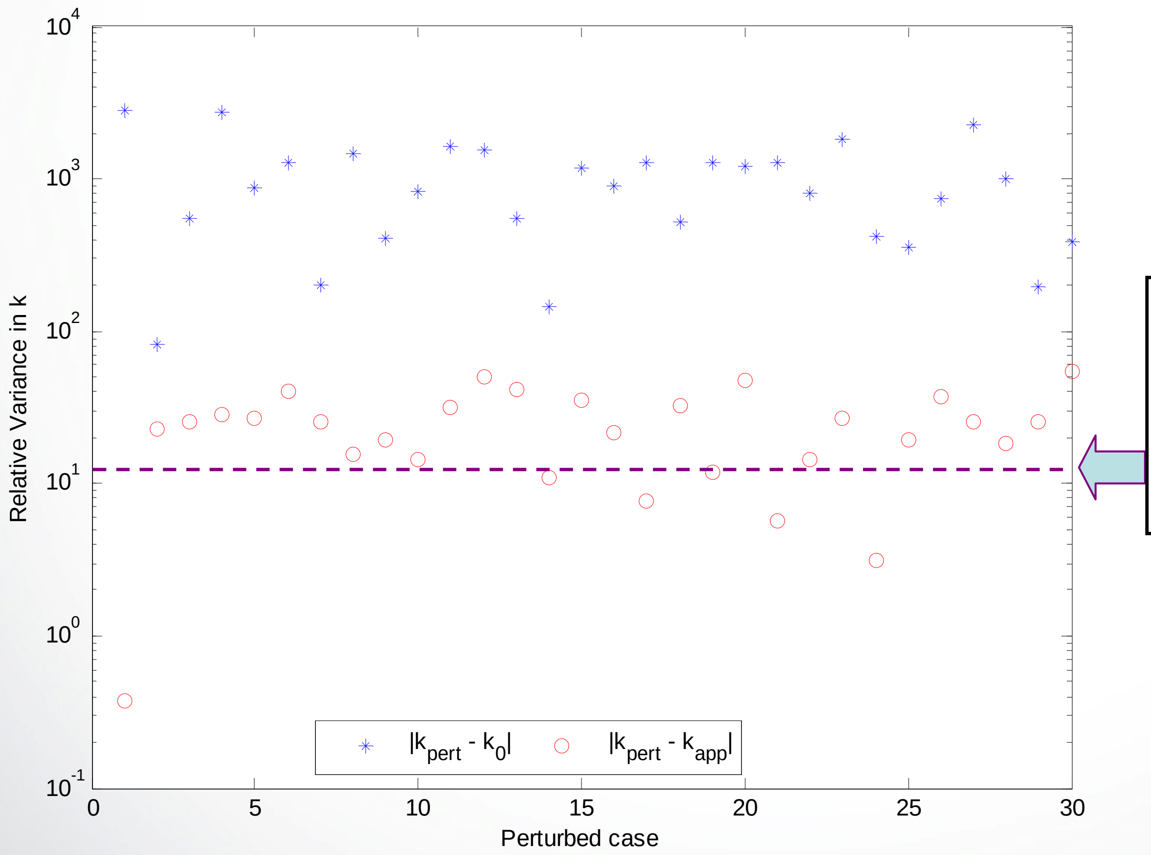
$$= k\left[\vec{\sigma}_0 + \left(\mathbf{Q}_r \mathbf{Q}_r^T\right)\Delta\vec{\sigma}\right]$$



The range r is found: ***r* = 619** .

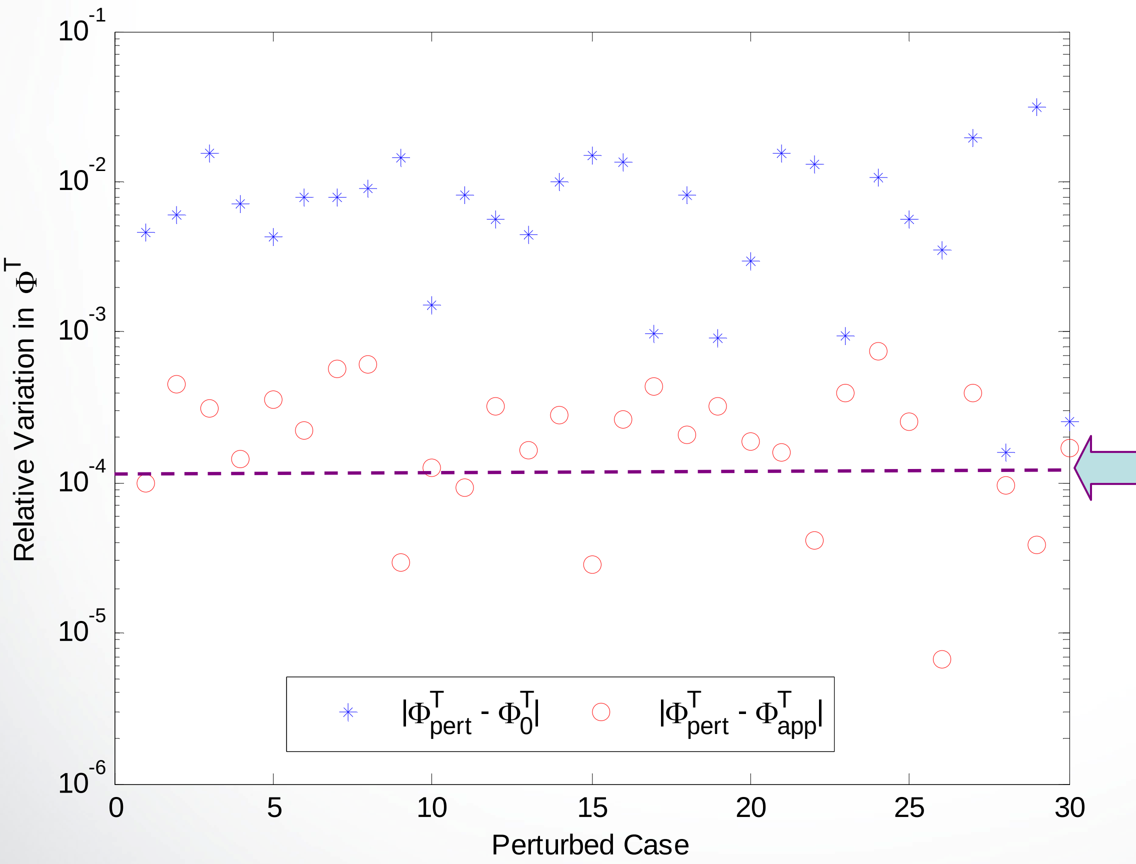
Recall ***n* = 68306**, so ***r* << *n***.

GPT-Free Error for *k* Eigenvalue



Statistical uncertainty level of *k* eigenvalue.

GPT-Free Errors for Thermal Flux



Statistical uncertainty level of thermal flux.

Conclusions & Perspectives

- GPT-Free method is successfully applied to a Monte Carlo based BWR model to enable sensitivity analysis of generalized responses.
- A reduced order model approach is employed to reduce the number of effective input parameters in order to simplify forward sensitivity analysis procedure.
- Ongoing work is focusing on extending this methodology to include depletion effects and nonlinear response variations in nuclear reactor analysis.
- [ANS-San Diego]: New developments indicate that the sensitivity subspace for GPT-free method in Monte Carlo models can be obtained with significantly reduced efforts than regular MC simulations. This is possible by taking advantages of the independence of epistemic and aleatoric uncertainties.

Questions?