Nuclear Data Sensitivity Analysis in OpenMC Using the GPT-Free Method

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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 in **Uncertainty Quantification (UQ)** procedure.
- **Forward Sensitivity Analysis (FSA)** is efficient if the number of responses of interest (outputs) in the problem considerably exceeds the number of parameters (inputs), while **Adjoint Sensitivity Analysis (ASA)** is advantageous for systems with a large number of parameters.
- **Deterministic** models are generally advantageous in 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, 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 *k* eigenvalue due to perturbed cross-sections in reactor analysis.
- **GPT** expands PT to determine variations of generalized formulation of responses, e.g. the ratios of different responses.
- Both **PT** and **GPT** provide an efficient tool to calculate sensitivities in various applications, particularly for deterministic models

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, **a general extension** of GPT theory in Monte Carlo method is not straightforward and takes certain amount of additional efforts.

GPT-Free: Overview

- **Objectives** of the GPT-free method:
  - Generate sensitivity profiles of generalized responses of interest with respect to input parameters **by precluding the 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 formulated as an unknown function of the state-space (neutron flux), $\boldsymbol{\phi}$**

$$k = f(\phi)$$

2. **Consider a response functional that is an inner product of some cross-sections, $\boldsymbol{\sigma}$, and the flux, $\boldsymbol{\phi}$**

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

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

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

4. **Differentiate with respect to cross-sections**

Fundamental Sensitivity Profile

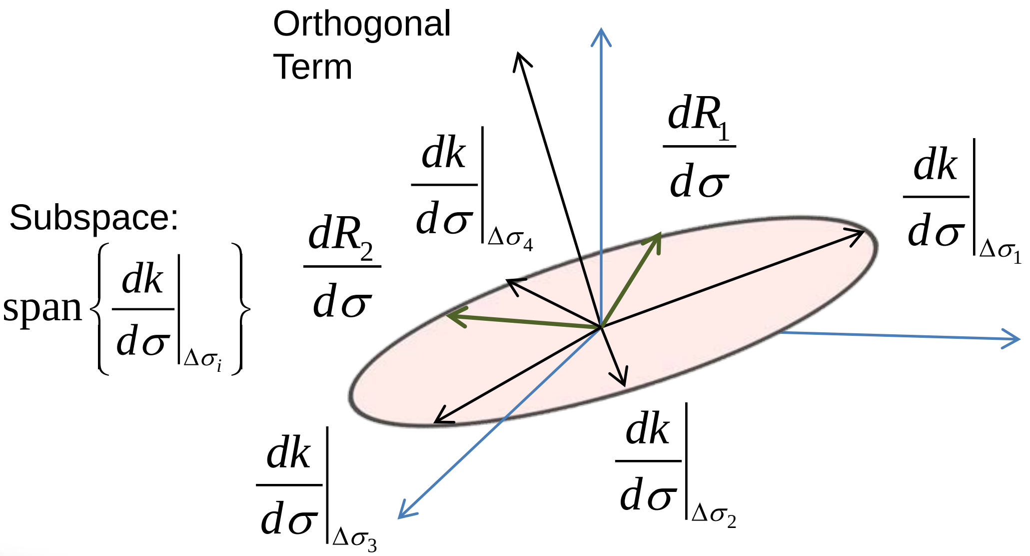
$$\frac{dk}{d\sigma} = \sum_{i=1}^{m} \frac{\partial f}{\partial R_i} \frac{dR_i}{d\sigma}$$

General Response Sensitivity Profiles

Constructing Equivalent Subspace

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

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

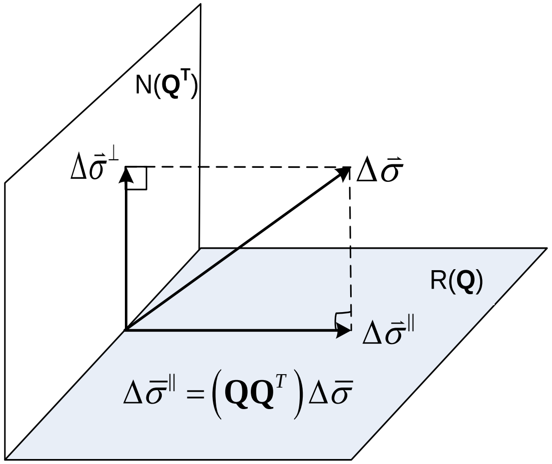


Project Parameter Perturbation onto Sensitivity Subspace

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

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

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



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

Forward SA (FSA) and ROM Technique

- The key step in forward **SA** is to obtain the response variation: $f\left(\vec{\sigma}_0+\Delta\vec{\sigma}\right)$
- **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, $f\left(\vec{\sigma}_0+\Delta\vec{\sigma}\right)\approx f\left(\vec{\sigma}_0+\Delta\vec{\sigma}^{\parallel}\right)$

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

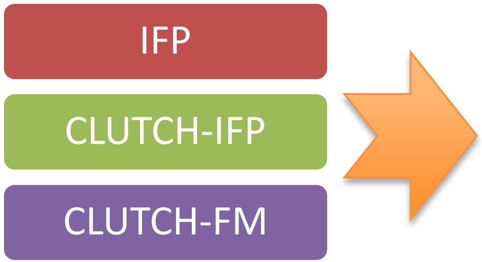
  This procedure requires only ***r*** forward executions.

***r* << *n* !!!**

GPT-Free Application in OpenMC

Status of the OpenMC SA Capabilities

- OpenMC is a modern, open source Monte Carlo particle transport code developed at MIT: https://github.com/mit-crpg/openmc.
- Continuous-energy sensitivity analysis capability was recently integrated in OpenMC for both eigenvalue and generalized sensitivity coefficient problems.
- The IFP (iterated fission probability) and CLUTCH methods were implemented for adjoint and generalized adjoint calculation
  - For CLUTCH, importance distribution can be provided by IFP or FM (fission matrix) method



PT

$$S_{k,\sigma} = \frac{\delta k / k}{\delta \sigma / \sigma} = \sigma \frac{\left\langle \Phi^*, \left(\frac{1}{k} \frac{\delta F}{\delta \sigma} - \frac{\delta L}{\delta \sigma} \right) \Phi \right\rangle}{\left\langle \Phi^*, \frac{1}{k} \mathbf{F} \Phi \right\rangle}$$

GPT

$$S_{R,\sigma} = \frac{\delta R / R}{\delta \sigma / \sigma} = \frac{\delta \Sigma_1 \Phi}{\langle \Sigma_1, \Phi \rangle} - \frac{\delta \Sigma_2 \Phi}{\langle \Sigma_2, \Phi \rangle} + \left\langle \Gamma^*, \left(\frac{1}{k} \frac{\delta F}{\delta \sigma} - \frac{\delta L}{\delta \sigma} \right) \Phi \right\rangle$$

$$R = \frac{\langle \Sigma_1, \Phi \rangle}{\langle \Sigma_2, \Phi \rangle}$$

Implementation of GPT-Free in OpenMC

ROM Determination

1. Generate *many* cross section perturbations
   - Adding Gaussian distribution noises to groups
2. OpenMC *k*-sensitivity calculations
   - Group-wise coefficients using IFP approach
3. Identify sensitivity subspace
   - Range finding algorithm to find

$$\vec{\sigma}_{pert,i} = \vec{\sigma}_0 + \Delta\vec{\sigma}_i$$

$$\vec{z}_i = \left.\frac{dk}{d\vec{\sigma}}\right|_{\vec{\sigma}_{pert,i}} \in \mathbb{R}^n \qquad \mathbb{Z} = [\vec{z}_1, \vec{z}_2, \ldots, \vec{z}_p] \in \mathbb{R}^{n\times p}$$

$$\mathbb{Z} = qr(\mathbf{Q}_r, \mathbf{R}_r), \quad \mathbf{R}_r \in \mathbb{R}^{r\times r} \text{ and } \mathbf{Q}_r \in \mathbb{R}^{n\times r}$$

$$\left\| \mathbb{Z} - \mathbf{Q}_r\mathbf{R}_r \right\| < \varepsilon$$

Sensitivity Analysis

4. Generate *r* cross section perturbations
   - Adding Gaussian distribution noises to groups
5. OpenMC forward calculations
   - Tally the responses
6. Evaluate response sensitivity
   - Utilize the sensitivity subspace

$$\vec{\sigma}_{pert,i} = \vec{\sigma}_0 + \Delta\vec{\sigma}_i^{\parallel} = \vec{\sigma}_0 + \left(\mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\vec{\sigma}_i$$

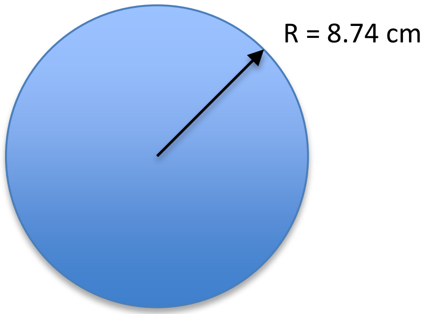
$$\Delta R_i = R(\vec{\sigma}_0 + \Delta\vec{\sigma}_i^{\parallel}) - R(\vec{\sigma}_0), \; i = 1,\ldots,r$$

$$\frac{dR}{d\vec{\sigma}} = \mathbf{Q}_r(\mathbf{\Gamma}^T)^{\dagger}\Delta\vec{\mathbf{R}}$$

$$\mathbf{\Gamma} = [\vec{\gamma}_1, \ldots, \vec{\gamma}_r], \quad \vec{\gamma}_i = \mathbf{Q}_r^T\Delta\vec{\sigma}_i, \; i = 1,\ldots,r$$

Case Problem

- Godiva criticality benchmark model (HEU-MET-FAST-001)



Highly enriched uranium (94 wt.%)

Density (g/cc)	18.74
Isotope	Atom density (atom/b-cm)
U234	4.9184e-04
U235	4.4994e-02
U238	2.4984e-03

44-group structure for perturbation and sensitivity profile calculations on fission cross section of U-235

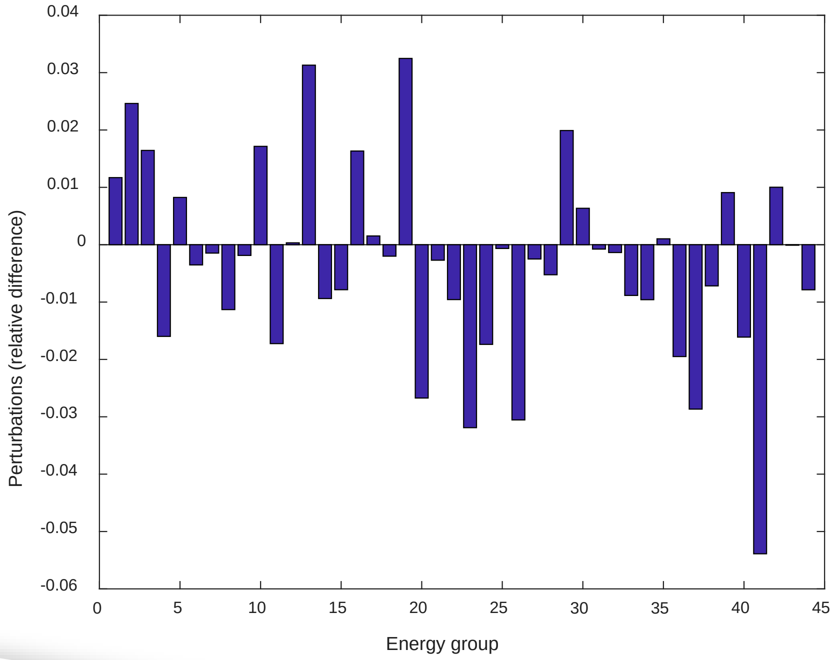
Response

$$R = \frac{\Sigma_f^{238\mathrm{U}}\phi}{\Sigma_f^{235\mathrm{U}}\phi}$$

PT: *k*-sensitivity: **IFP**
GPT: *R*-sensitivity: **CLUTCH-FM**

Results (1/5)

- One cross-section perturbation: 2% Gaussian distribution relative noise.



Results (2/5)

- *k*-sensitivity calculation: *n* = 100 perturbations

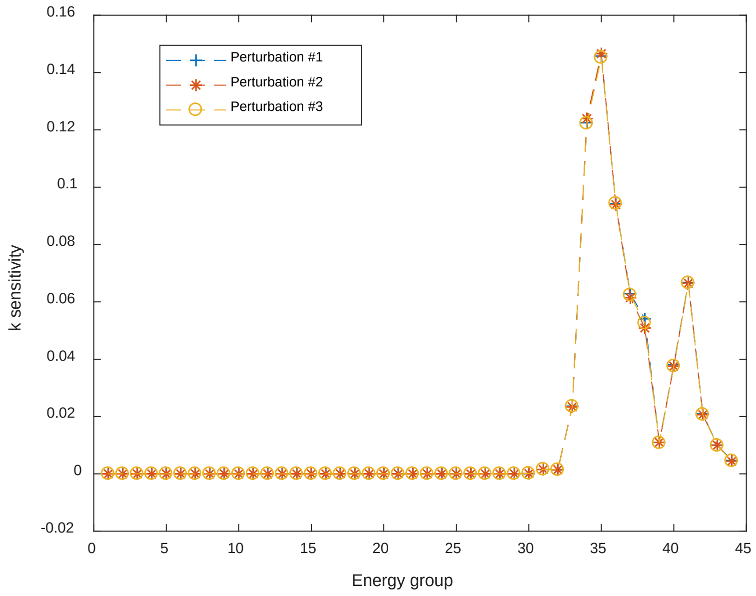
$$\mathbb{Z}=[\left.\frac{dk}{d\vec{\sigma}}\right|_{\vec{\sigma}_{pert,1}},\left.\frac{dk}{d\vec{\sigma}}\right|_{\vec{\sigma}_{pert,2}},\ldots,\left.\frac{dk}{d\vec{\sigma}}\right|_{\vec{\sigma}_{pert,100}}]\in\mathbb{R}^{44\times100}$$

$$[\mathbf{Q},\mathbf{R}]=qrsovle(\mathbb{Z})$$

$$r=12$$

$$\mathbf{Q}_r=\mathbf{Q}(:,1:r),\mathbf{R}_r=\mathbf{R}(:,1:r)$$

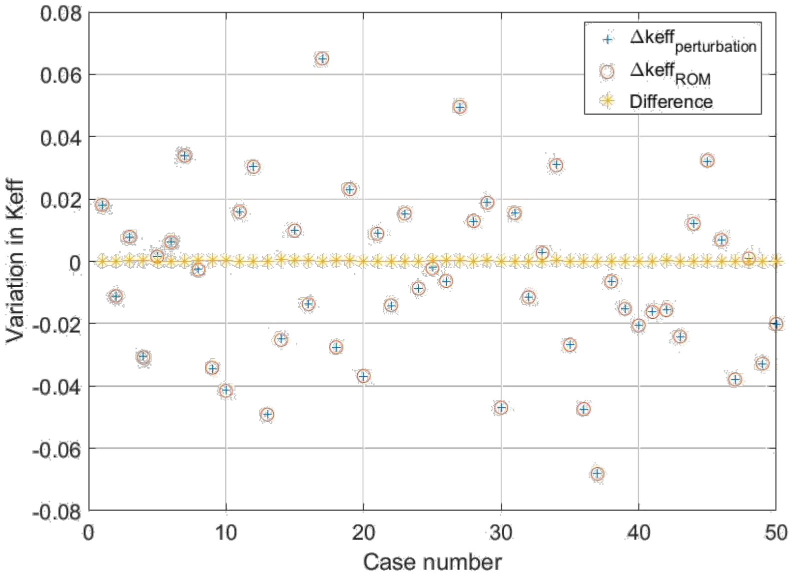
$$\left\|\mathbb{Z}-\mathbf{Q}_r\mathbf{R}_r\right\|<10^{-3}$$



Results (3/5)

- **Validation of the ROM with *k* eigenvalue perturbations**

Perturbing cross section using ROM with r = 12.

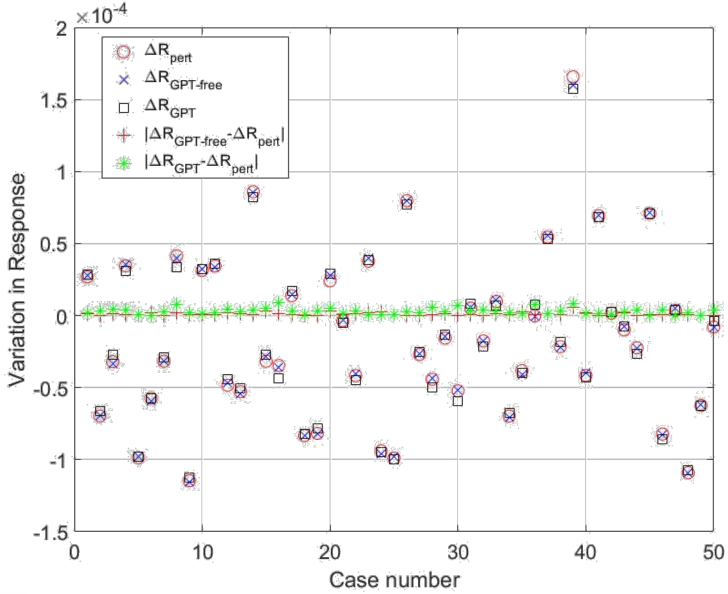


$$\Delta\vec{\sigma}^{\parallel} = (\mathbf{Q}_r \mathbf{Q}_r^T)\Delta\vec{\sigma}$$

$$k(\vec{\sigma}_0 + \Delta\vec{\sigma}^{\parallel}) \approx k(\vec{\sigma}_0 + \Delta\vec{\sigma})$$

Results (4/5)

- GPT-free accuracy for a general response variations



Response

$$R = \frac{\Sigma_f^{^{238}\mathrm{U}} \phi}{\Sigma_f^{^{235}\mathrm{U}} \phi}$$

Reference

$$\Delta R_{\mathrm{pert}} = R(\vec{\sigma}_0 + \Delta\vec{\sigma}^{\parallel}) - R(\vec{\sigma}_0)$$

SA calculation

$$\Delta R_{SA} = \left(\frac{dR}{d\vec{\sigma}}\right)^T \cdot \Delta\vec{\sigma}$$

Results (5/5)

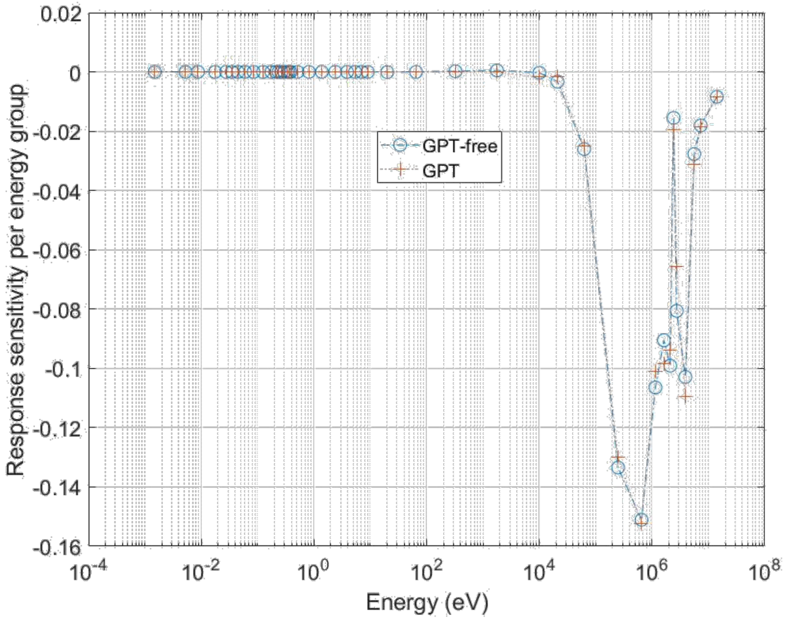
- **Group-wised response sensitivity comparison between GPT and GPT-free**

GPT-free response sensitivity

$$\frac{dR}{d\vec{\sigma}} = \mathbf{Q}_r(\mathbf{\Gamma}^T)^\dagger \Delta\vec{\mathbf{R}}$$

$$\mathbf{\Gamma} = [\vec{\gamma}_1, \ldots, \vec{\gamma}_K]$$

$$\vec{\gamma}_i = \mathbf{Q}_r^T \Delta\vec{\sigma}_i, \ i = 1, \ldots, N$$



Result Discussion

- The k_{eff} variations, general response variations, and group-wised sensitivities predicted by the ROM GPT-free approach all agree quite well with reference results, proving an effective rank nearly captures the dominant directions of cross-sections variations.
- It is also observed the GPT-free results are even closer to the reference perturbation values as compared to the standard GPT method, implying that the active subspace captures the directions that are responsible for both linear and nonlinear behaviors. In other words, GPT-free overcomes the accuracy limit restrained on GPT.

Summary

- GPT-free method is implemented in OpenMC for evaluation of the nuclear data sensitivity coefficients.
- The applicability of GPT-free method is demonstrated by calculating response sensitivities using the Godiva benchmark model.
- The accuracy of the approach, particularly on the calculation of energy-dependent response sensitivity, is directly verified by the GPT sensitivity analysis capability of OpenMC.
- Further investigation will focus on examining the efficiency of GPT-free approach with more practical problems as well as extending its applications to other problems such as depletion perturbation problems.

Thank you for your time!