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Further Developments of GPT-Free Sensitivity Analysis in Multi-Group Monte Carlo Models

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Introduction

- **Sensitivity Analysis (SA)** determines the most influential components in the input parameters corresponding to the output responses, meanwhile it can provide valuable information to facilitate **Uncertainty Quantification (UQ)** procedure.
- **Perturbation theory (PT)** and **Generalized perturbation** theory **(GPT)** provides an efficient tools to estimate response sensitivities in nuclear reactor calculations for decades.
- Recently a forward based **GPT-Free** method is introduced and intended to perform response sensitivity analysis without the need to solve adjoint equations associated with **GPT** applications.
- GPT-Free method has been successfully implemented to both **deterministic** and **Monte Carlo** modeling problems and results shown in previous ANS meetings verifies its feasibility and efficiency.

Generalized Perturbation Theory (GPT)

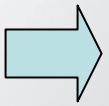
- The adjoint formulation in traditional perturbation theory (PT) enables one to efficiently predict the change in eigenvalue k due to nuclear parameter perturbs in reactor analysis.
- GPT expands PT to determine variations of generalized responses, e.g. bilinear ratios of responses.
- Both PT and GPT 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.

GPT-free method is developed to address these limitations.



GPT-Free: Theory

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

$$k = f(\phi)$$

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

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

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

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

4. Differentiate with respect to cross-sections

Fundamental Sensitivity Profile

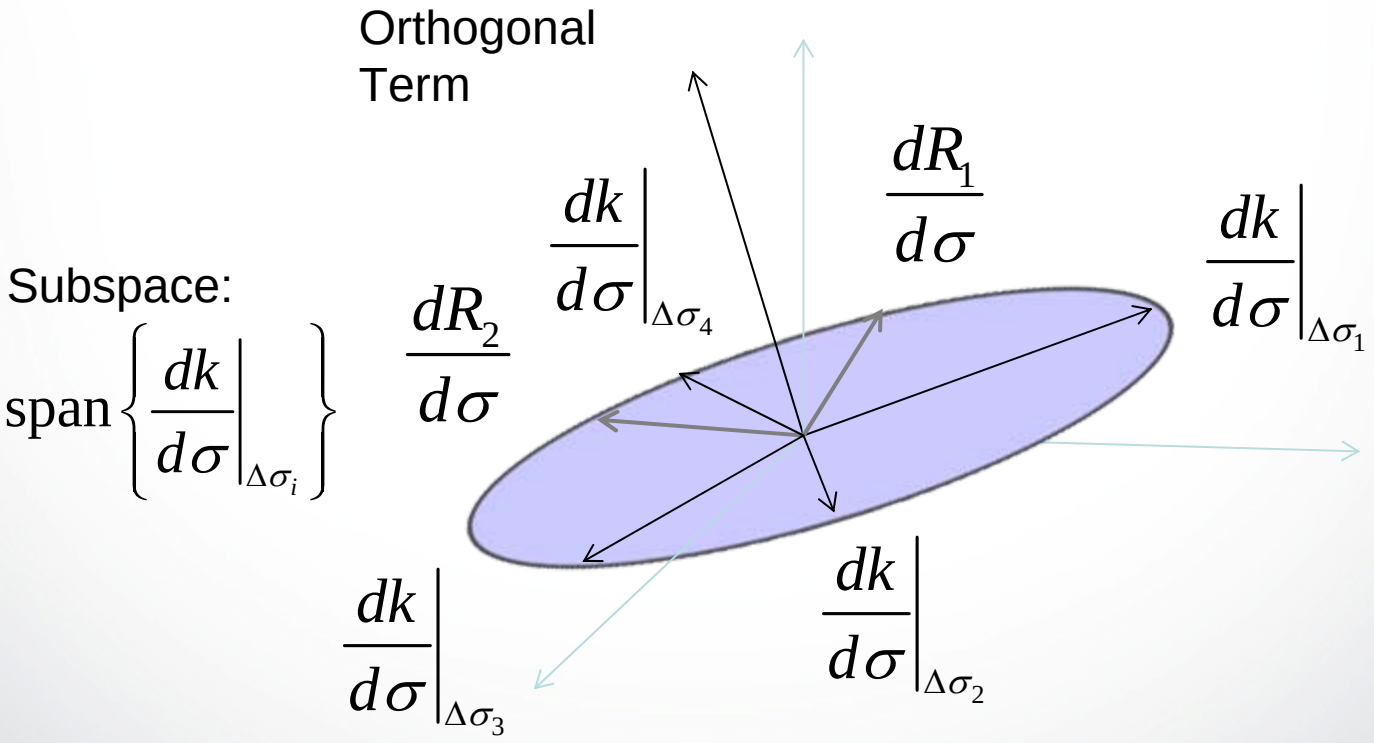
$$\frac{dk}{d\sigma} = \sum_{i=1}^{m} \frac{\partial f}{\partial R_i} \frac{dR_i}{d\sigma}$$

General Response Sensitivity Profiles

Constructing Active Subspace

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

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

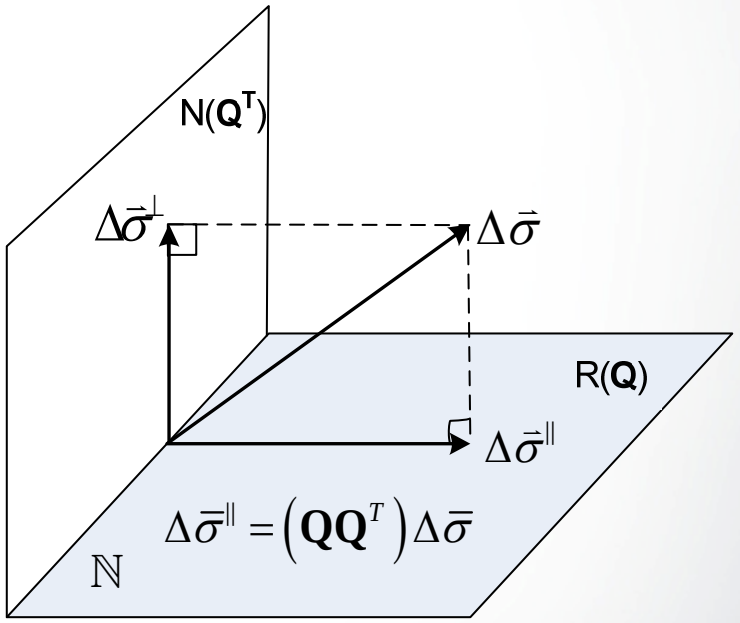


Project Parameter Perturbation onto Sensitivity Subspace

Let $\mathbb{N}$ denote the active 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: $\Delta\vec{\sigma}^{\|}=\left(\mathbf{Q}_r\mathbf{Q}_r^T\right)\Delta\vec{\sigma}=\sum_{i=1}^{r}\vec{q}_i\left(\vec{q}_i^T\Delta\vec{\sigma}\right)=\sum_{i=1}^{r}\alpha_i\vec{q}_i$

  Then,

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

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

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

r << n !!!

Advantages of GPT-Free Method

- Preclude GPT-based adjoint calculation
- Reduce order model (ROM) operate on input parameter level
- Easy to extend from deterministic (DT) models to Monte Carlo (MC) models

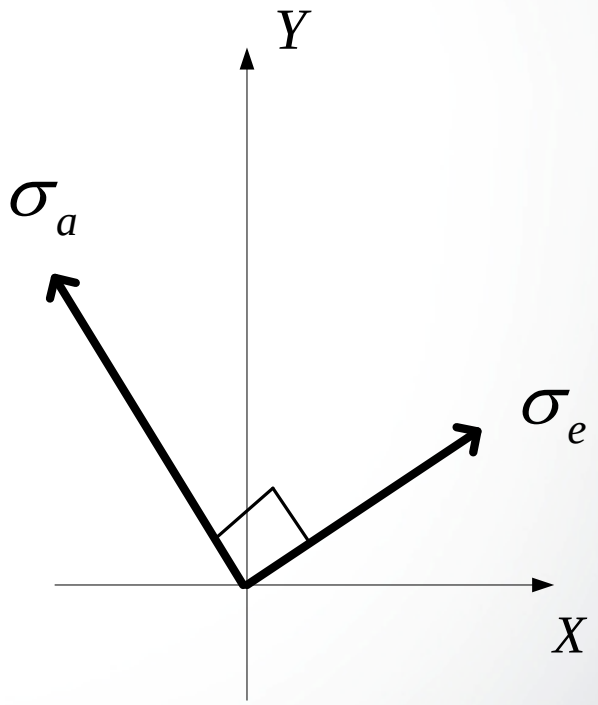
Difficulties in Current GPT-Free Method

- For typical reactor models with sufficient details, the dimension of the reduced subspace for nuclear data (i.e., cross sections) is found to be in the order of several hundreds (example will be presented later).
- Several hundred forward runs are required to generate complete sensitivity profiles of all responses with respect to all cross sections.
- The procedure to construct the active sensitivity subspace in GPT-Free method is also turned out to be computational costly, especially for Monte Carlo models.

Time, Time, Time !!!

Background of Proposed Approach

- Epistemic vs. Aleatoric uncertainty
- Two uncertainties are reduced by distinct strategies
- Independence of the two uncertainties



Independnce of σ_a and σ_e

Implementation of Proposed Approach

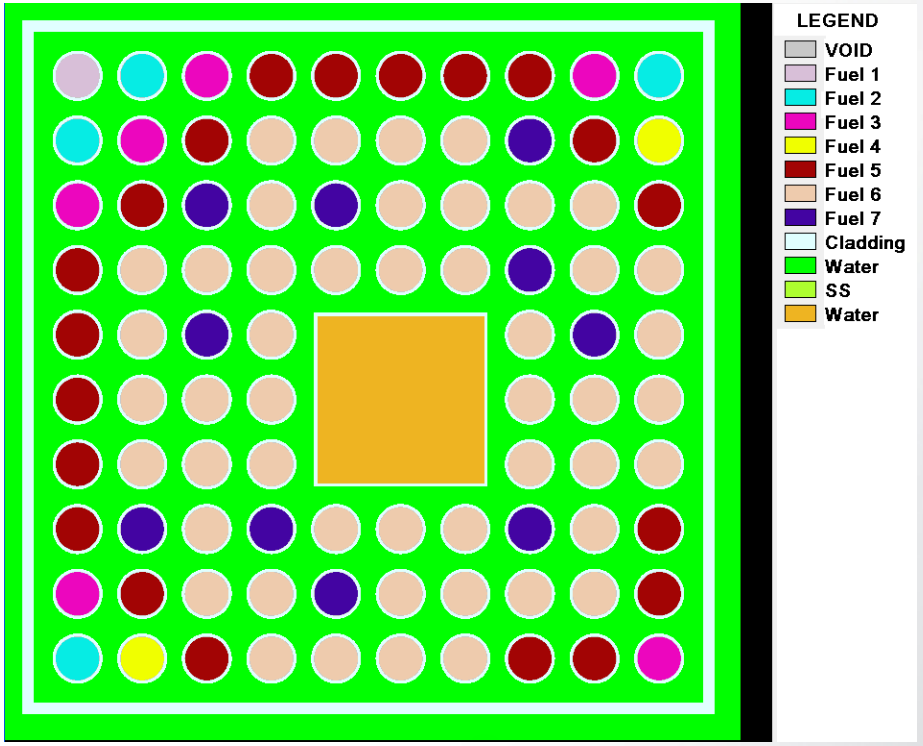
1. Perform reference MC simulation with enough number of particle histories to reach the desired level of statistical uncertainties.
2. Perform *n* MC simulations using a much smaller number of particle histories used in step 1, wherein each simulation the cross-sections are randomly perturbed in a statistically 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.
3. Identify the active sensitivity subspace in a similar manner to the current GPT-Free algorithm, and determine effective rank *r* of the subspace via a rank finding algorithm.
4. Perform forward sensitivity analysis based on the subspace and effect rank obtained from step 2 and 3.
5. End.

Simplified!

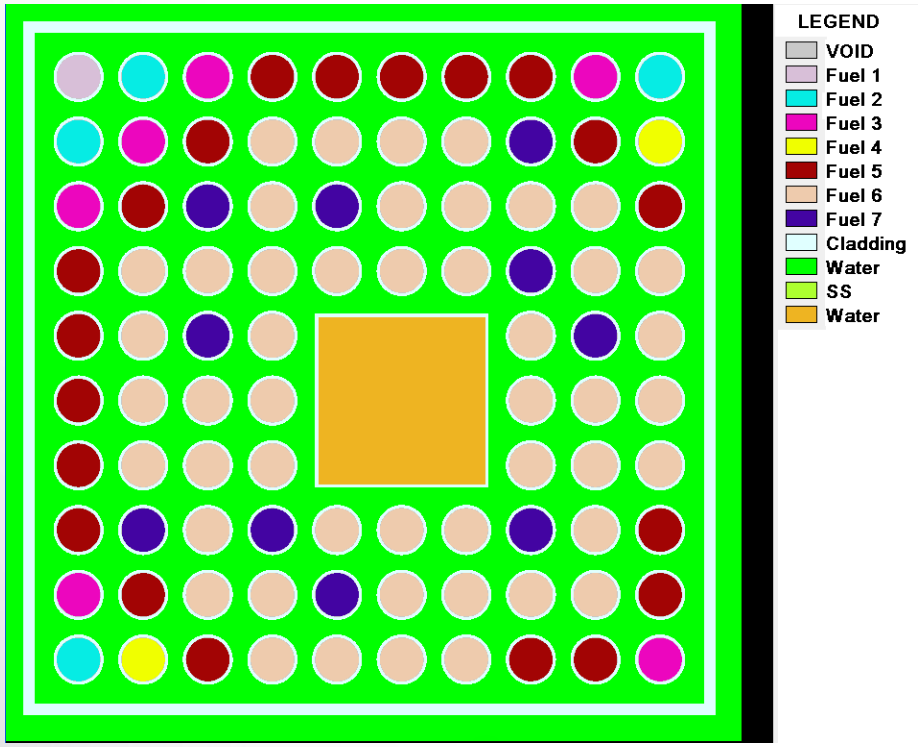
Case Study

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)

1. Randomly perturb cross sections $\bar{\sigma}_{\text{pert},i} = \bar{\sigma}_0 + \Delta\bar{\sigma}_i$

2. Execute the sensitivity analysis sequence in SCALE to calculate $dk/d\bar{\sigma}\big|_i$

3. Repeat *r* times and form the decomposition:

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

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

Simplified!

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

The κ-Metric for Eigenvalue

The κ-metric is defined as:

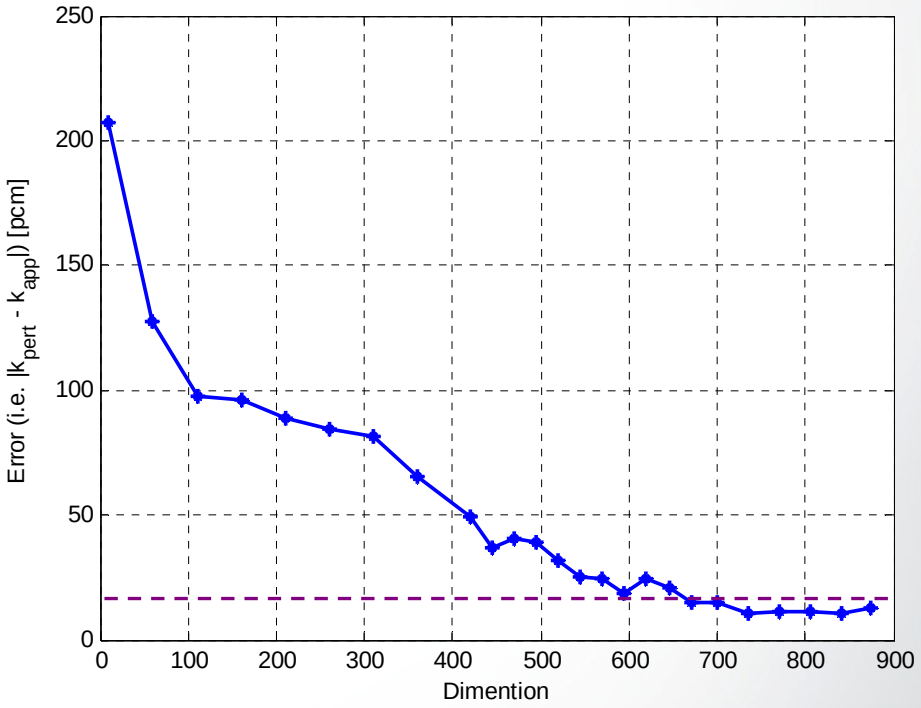
$$\kappa = \left| k_{\text{pert}} - k_{\text{app}} \right|$$

Where,

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

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

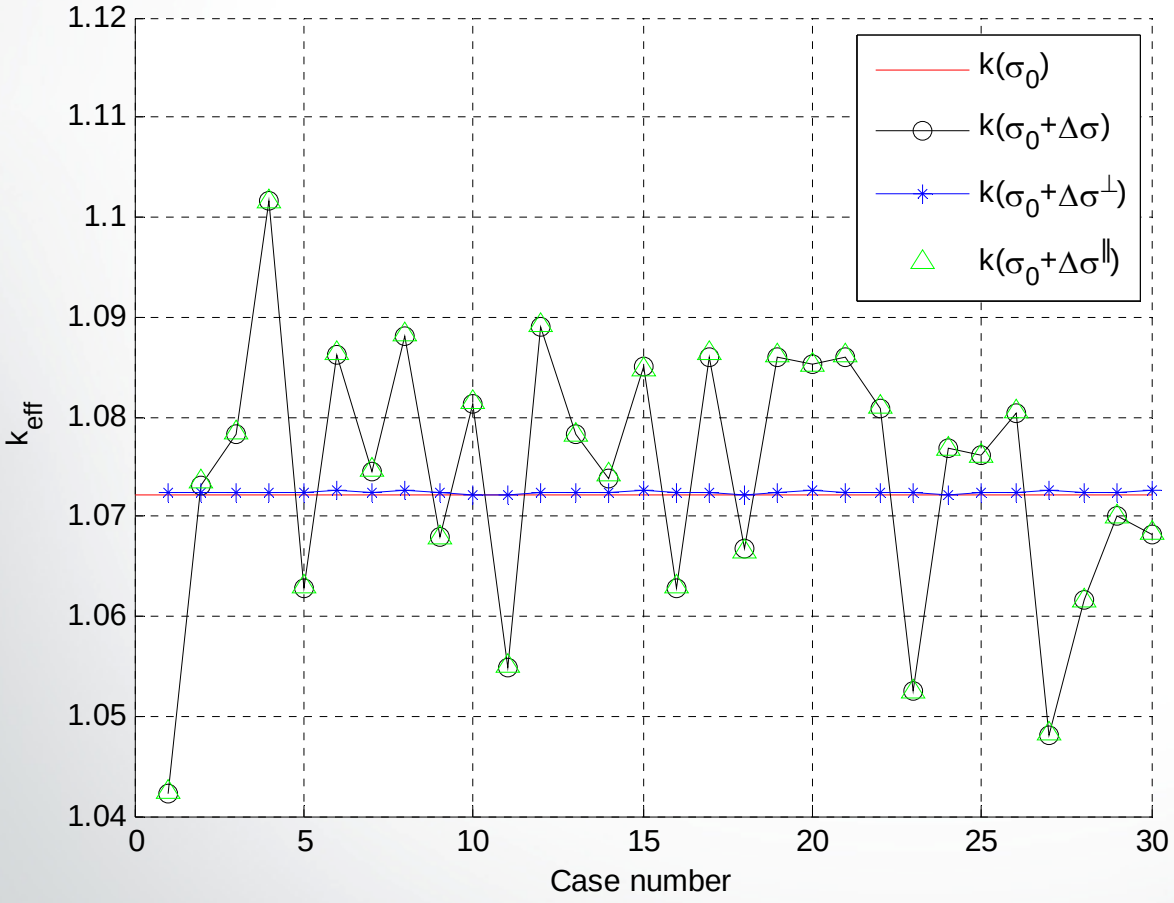
$$= k\left[\vec{\sigma}_0 + \left(\mathbf{Q}_r \mathbf{Q}_r^T\right)\Delta\vec{\sigma}\right]$$



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

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

Verification of Active Subspace via *k* Eigenvalue Response



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

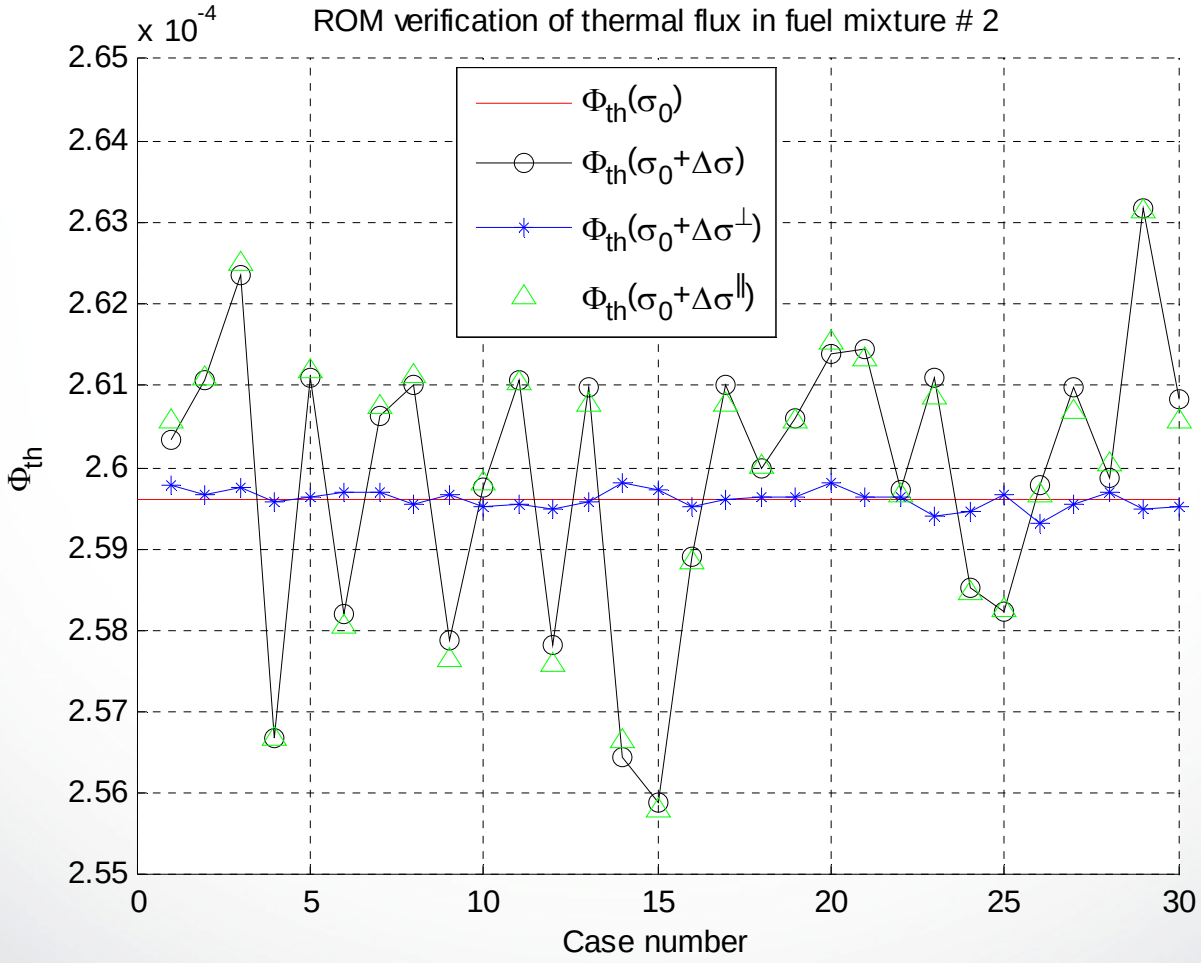
$$\Delta\sigma^{\parallel} = \left(\mathbf{Q}_r \mathbf{Q}_r^T\right)\Delta\sigma$$

The curves proves the identities:

$$k(\sigma_0 + \Delta\sigma^{\perp}) = k(\sigma_0)$$

$$k(\sigma_0 + \Delta\sigma^{\parallel}) = k(\sigma_0 + \Delta\sigma)$$

Verification of Active Subspace via Thermal Flux



Computing Time Required to Construct Active Sensitivity Subspace

	BEFORE	AFTER
Total Perturbations	619	619
Averaged Computing Time (min)	140.40	18.00
Total Computing Time (min)	86910.50	11143.70

Summaries & Perspectives

- The new approach of constructing active sensitivity subspace for GPT-free method in multi-group Monte Carlo models is developed and tested in a realistic BWR assembly calculations.
- The active sensitivity subspace can be constructed with significantly reduced efforts comparing to common treatment in previous work. The efficiency of the subspace is preserved via the verification process of various responses.
- [M&C 2013]: Most recent efforts on simplifying Monte Carlo forward calculation indicates more computation savings can be achieved on GPT-free sensitivity analysis procedure, again by taking advantages of the independence of epistemic and aleatoric uncertainties.