Advanced Research Activities in Nuclear Reactor Physics Calculations

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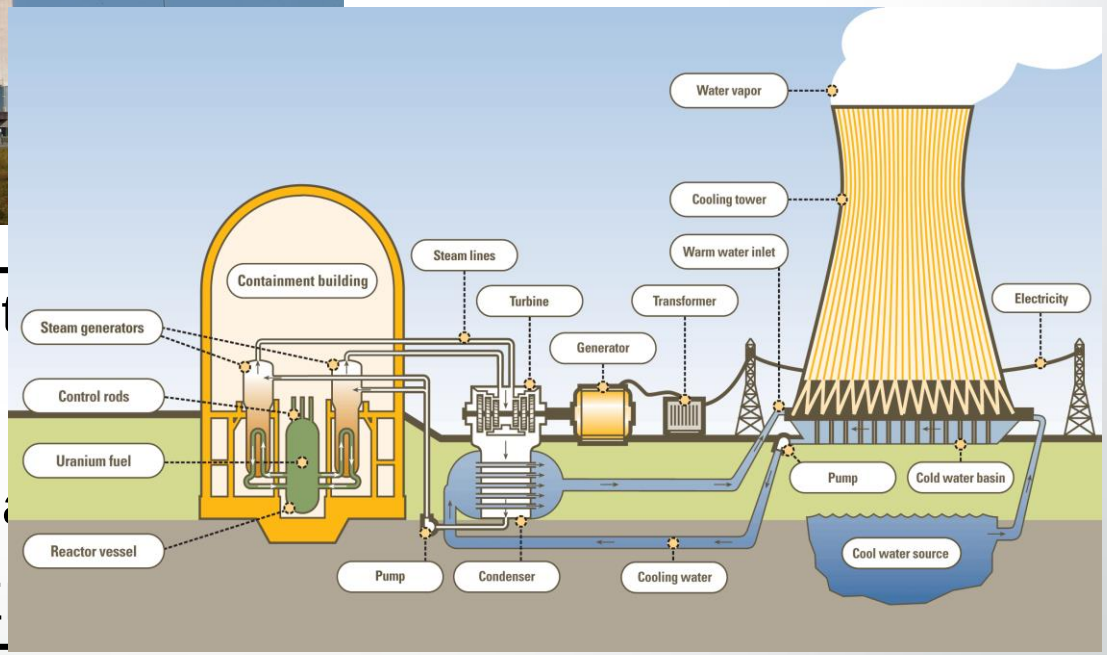
Outline

- Introduction
  - Nuclear reactor modeling and simulation (M&S)
  - Reactor physics calculation (Neutronics)
  - Sensitivity analysis and uncertainty quantification
- Research highlights
  - Hybrid Monte Carol - deterministic transport solutions
  - GPT-free sensitivity analysis method
- Summary

Introduction

Nuclear Reactor & Nuclear Power Plant

Schematic view of a typical PWR plant.



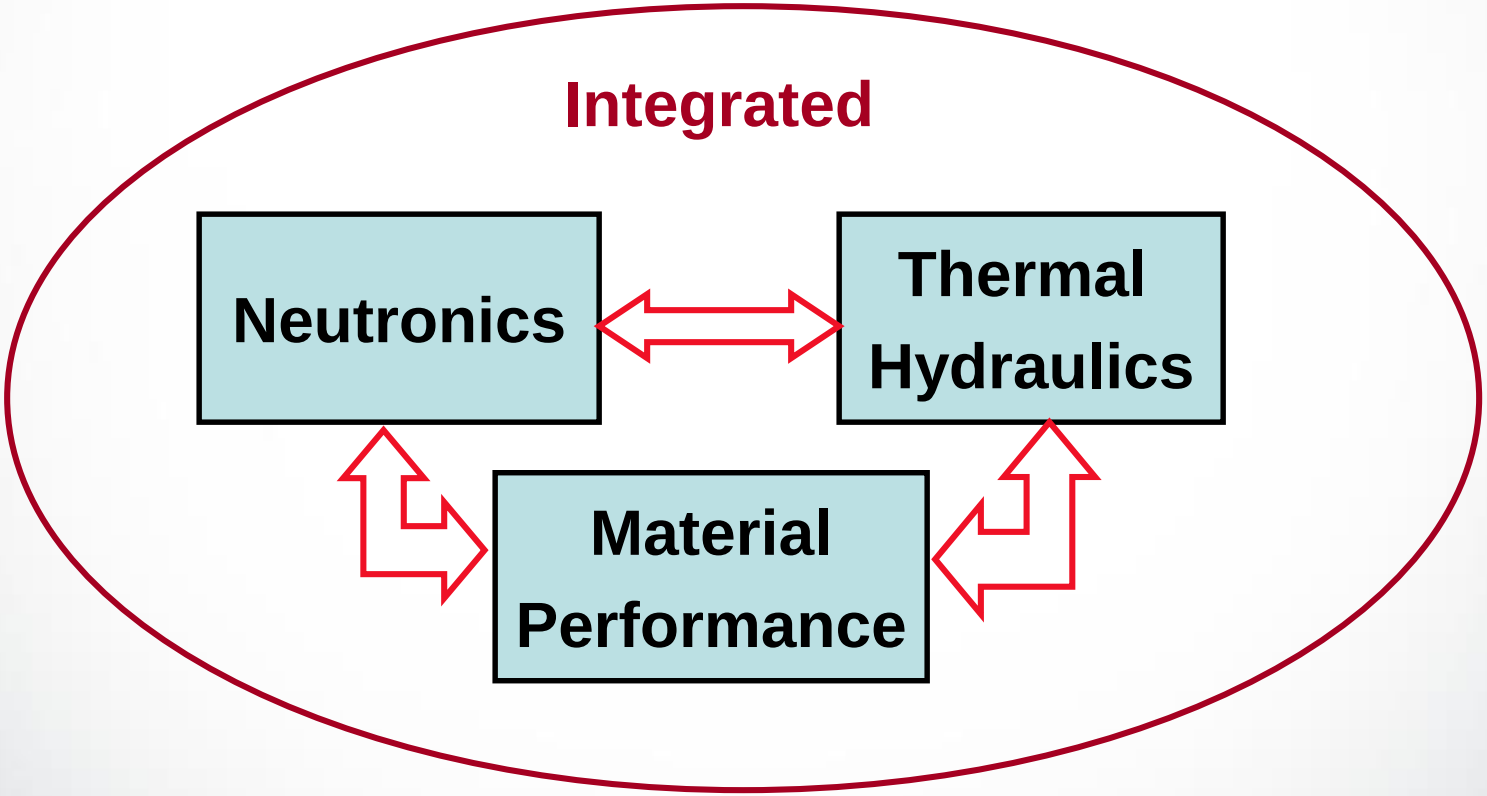
Total nuclear power plant unit

In operation: **435** (China: **16**)

Under construction: **62** (China

[By June 2012, courtesy of E

Reactor Modeling and Simulation (M&S)

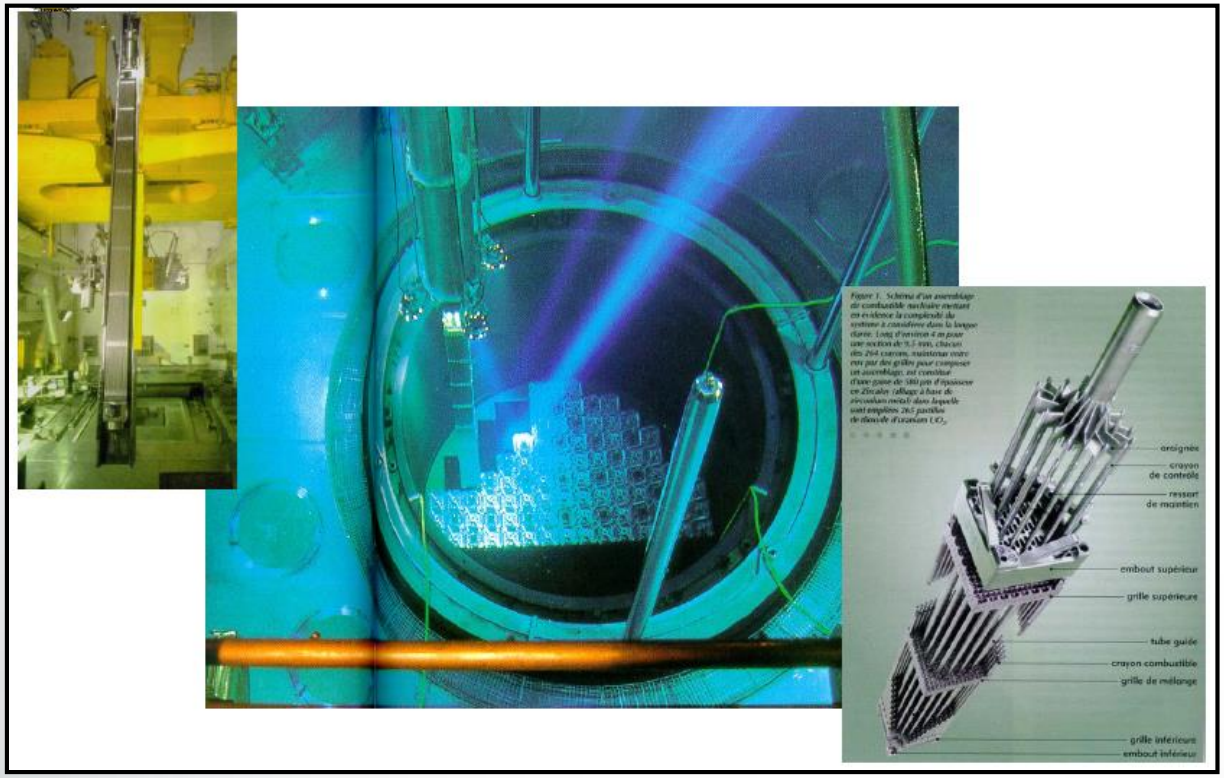


Uncertainty quantification reaches every components.

Major Concerns in M&S in Large Scale Reactor System

- Multi-Scale resolution
- Multi-Physics coupling
- Uncertainty management
- Integration technology
- High performance computing (HPC)

The Role of Neutronics Analysis



Example of a PWR core.

Neutronics aims to follow the neutron "economy" in a nuclear reactor in order to monitor and control the behavior of the fission chain reaction. (From Duderstadt & Hamiltion)

Difficulties Arose in Neutronics

- Geometry is challenging
  - 271 pins per assembly, about 400 assembly in core
  - 6 to 48 meshes per pin cell, 30 to 40 axial planes
  - About 10 to 100 millions of 3-D spatial meshes
- Physics is challenging
  - Varieties of neutron life cycle
  - Multi-physics coupling problem
  - Complexity in nuclide cross sections
  - Nuclear data sensitivities and uncertainties

Source of Uncertainties in Neutronics

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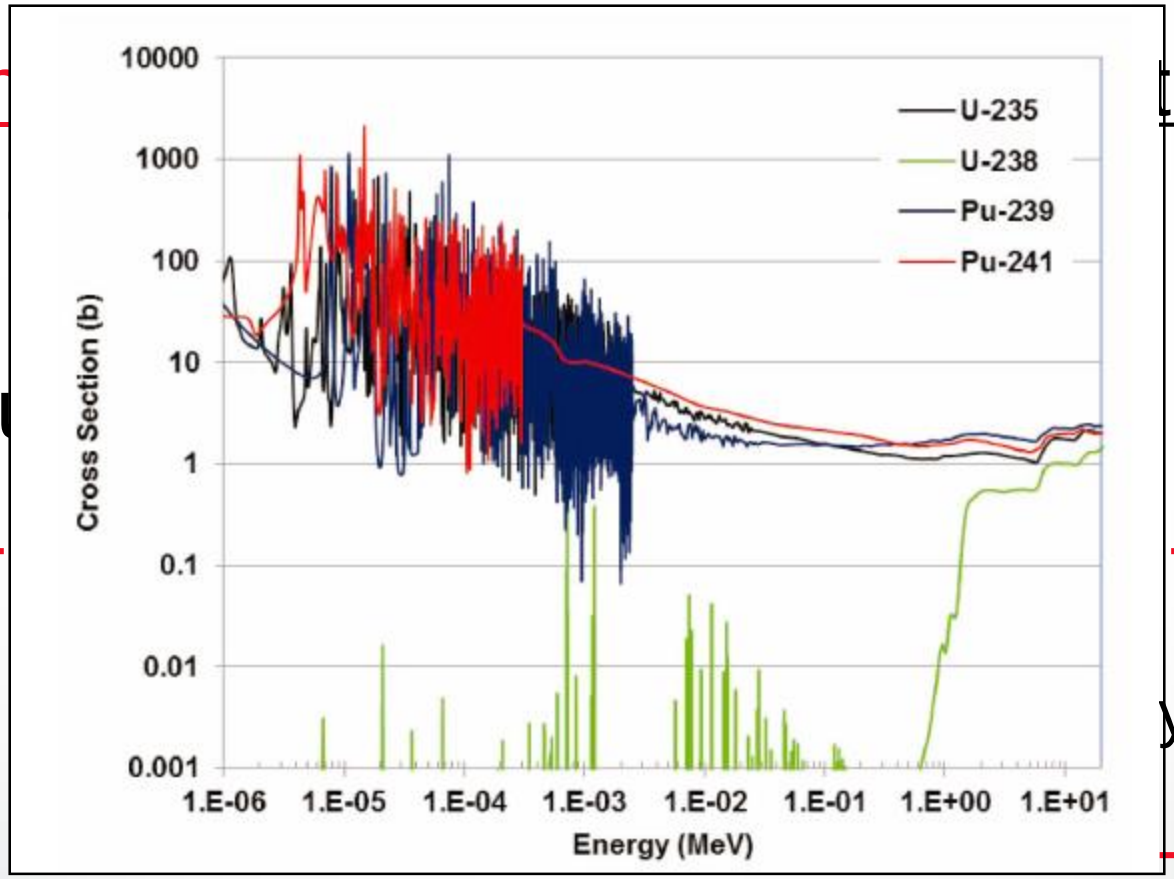

Energy dependent fission cross sections of U-235, U-238, Pu-239 and Pu-241.

Epistemic Uncertainty vs. Aleatoric Uncertainty

Tasks of Uncertainty Management

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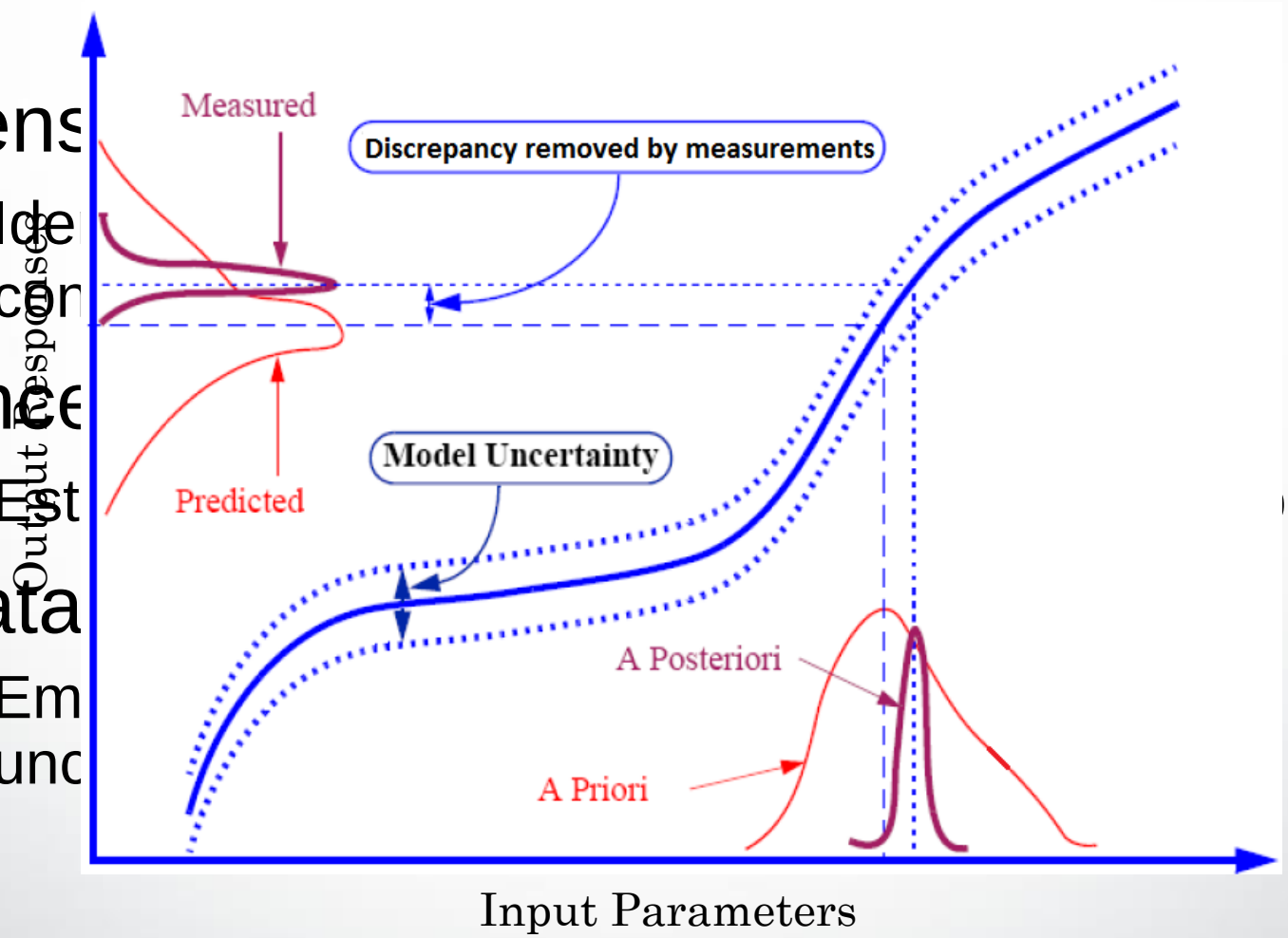


Hybrid Monte Carlo – Deterministic Transport Approaches

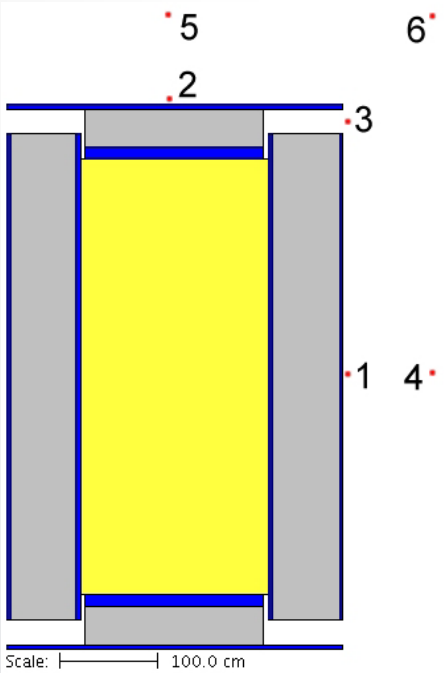
Introduction for Hybrid Approach

- Deterministic method is fast but lack of flexibility and inaccurate
- Monte-Carlo (MC) method is universal and more physical reliable but time consuming
- Hybrid deterministic-MC methods have being recently getting more and more interest to researchers.
- Deterministic models solution (both forward and adjoint) is employed to bias source particles and assign appropriate importance map to MC models to accelerate MC simulation and reduce the variance.
- Some current developed hybrid approaches:
  - Variational variance reduction (Densmore & Larsen 2003)
  - Correction method (Becker et al. 2007)
  - **FW-CADIS (Wagner et al. 2007)**
  - Talley linear combination (Solomon et al. 2009)
  - Coarse mesh finite difference (Lee et al. 2009)

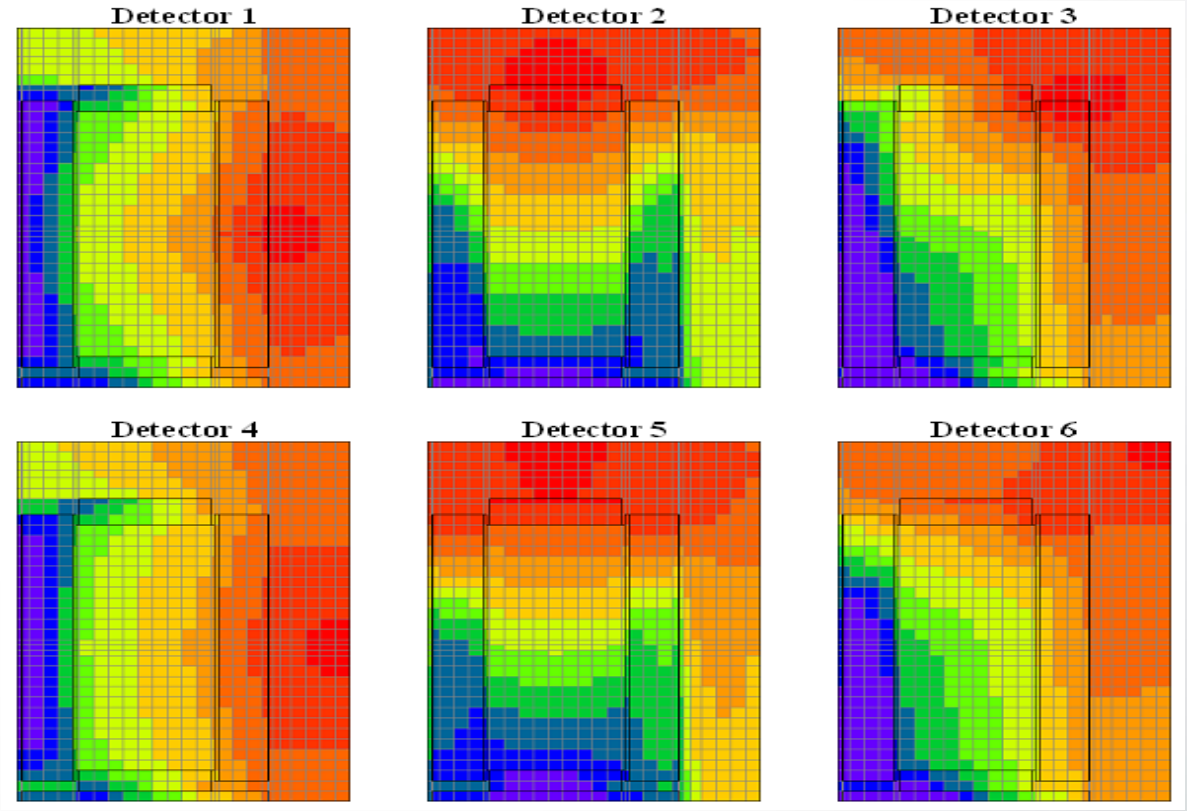
Current Challenges in Hybrid Approaches

- Multiple responses application
  - Importance for different responses are expected to be different
  - Adjoint calculation needs to perform individually for each response
  - Computational overheads become unacceptable with the increase of responses.
- Global and uniform variance reduction in the whole phase space

Adjoint Flux of Multiple Responses



Spent Fuel Cask with 6 Detectors



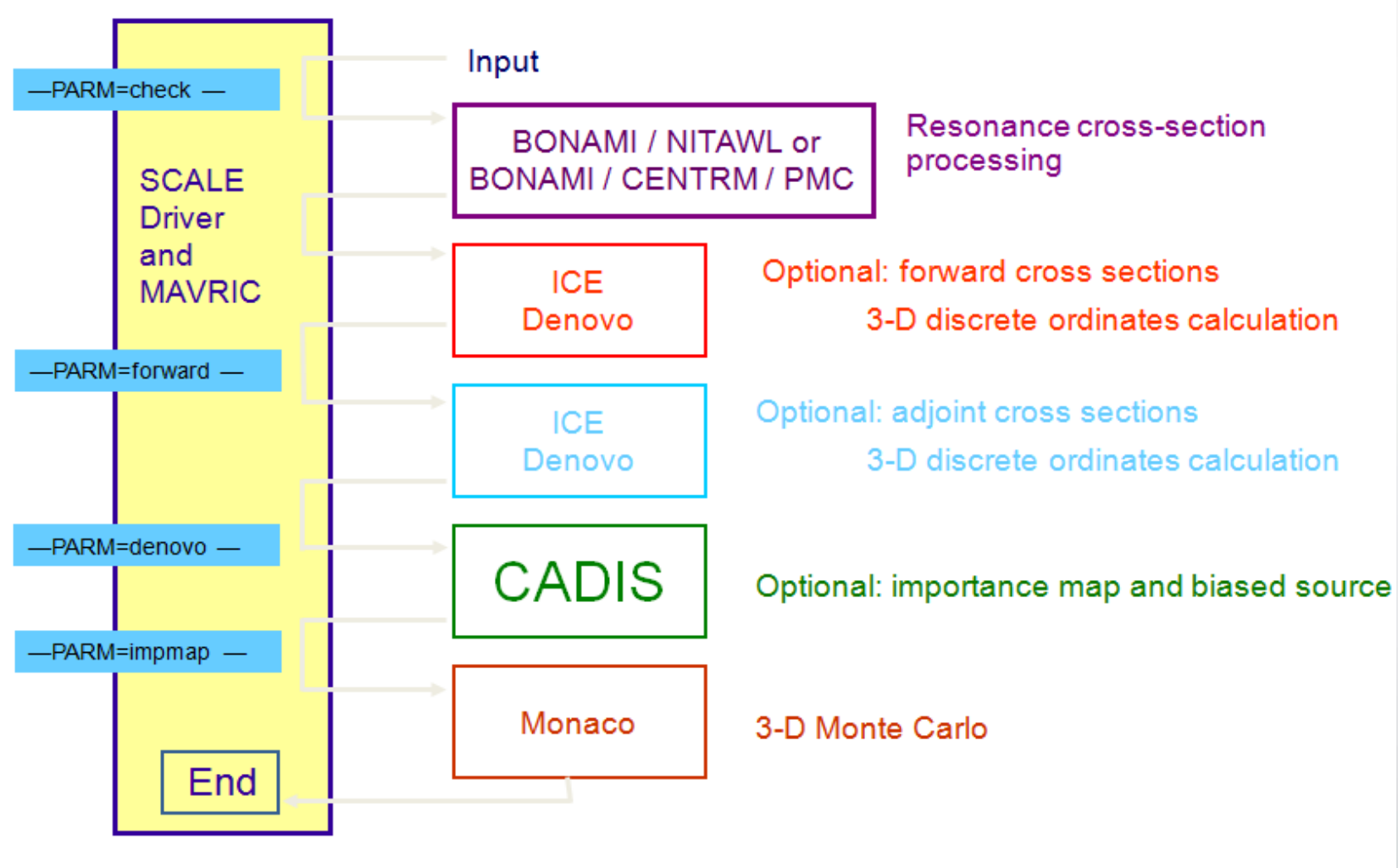
Corresponding Adjoint Flux Profiles

Outline of FW-CADIS Approach

- Adjoint deterministic model: $\mathbf{L}^*\left(\phi_i^*\right) = \frac{\partial R_i}{\partial \phi}$
- Adjoint solutions are employed to bias particle source distribution and weight window map
- Pseudo response - combine multiple responses with linear combination and the weight for each response is assigned as the reverse of the forward solutions

$$\xi = \sum_{i=1}^{m} R_i / \phi_i \quad \Rightarrow \quad \mathbf{L}^*\left(\phi^*\right) = \frac{\partial \xi}{\partial \phi}$$

FW-CADIS MAVRIC Sequence in SCALE



Fundamentals of the Proposed Approach

- Importance for different responses are expected to be correlated albeit they are different.
- Resulting responses uncertainties are expected to be correlated
  - Given *m* responses, let *r* denote number of independent correlations.
  - Each independent correlation is linear combination of original responses
  - Bias MC particles towards *r* (rather than *m*) independent correlations

Subspace approach is devised based on these ideas.

Subspace Approach - Estimating Single-Response-Importance (SRI) Matrix

Let R_i be the ith response, it may be described as

$$R_i = \langle \vec{\psi}, \vec{\sigma}_i \rangle, \text{ and } i = 1, \ldots, m$$

The importance map for R_i is obtained

$$L^* \vec{\psi}_i^* = \frac{\partial R_i}{\partial \vec{\psi}} = \vec{\sigma}_i$$

The Single-Response-Importance matrix is formed as

$$\mathbf{\Psi} = \begin{bmatrix} \vec{\psi}_i^* & \cdots & \vec{\psi}_m^* \end{bmatrix}$$

Correlations are identified by performing SVD on SRI matrix.

Outline of Subspace Approach

- Identify the correlations between weight window maps to minimize the computational time
- Form *r* pseudo response in Subspace approach

$$\xi_j^{\text{Subspace}} = \sum_{i=1}^{m} \alpha_{i,j} R_i, \quad j = 1, 2, \ldots, r$$

- Perform *r* MC calculations (with histories reduced) with weight window maps provided by

$$\mathbf{L}^*\left(\phi_j^*\right) = \frac{\partial \xi_j^{\text{Subspace}}}{\partial \phi}$$

- Estimate final solutions (mean and variance values) collectively as follows

$$\bar{x} = \sigma^2 \sum_{j=1}^{r} \frac{1}{\sigma_j^2} \bar{x}_j \quad \text{and} \quad \frac{1}{\sigma^2} = \sum_{j=1}^{r} \frac{1}{\sigma_j^2} \ .$$

Summary of Importance-based Biasing Approaches

- Deterministic Model:

$$\mathbf{L}^*\left(\phi_i^*\right) = \frac{\partial R_i}{\partial \phi}$$

- FW-CADIS:

$$\xi^{\text{FW-CADIS}} = \sum_{i=1}^{m} R_i / \phi_i \;\Rightarrow\; \mathbf{L}^*\left(\phi^*\right) = \frac{\partial \xi}{\partial \phi}$$

- Subspace Approach:

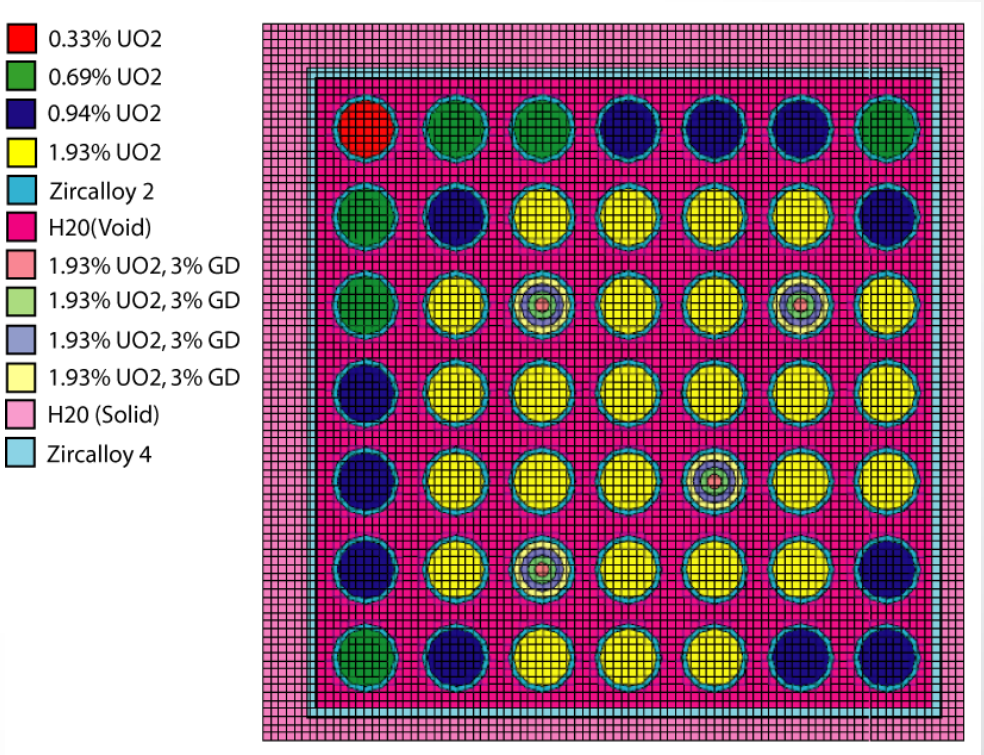
$$\xi_j^{\text{Subspace}} = \sum_{i=1}^{m} \alpha_{i,j} R_i, \quad j = 1,\ldots,r \;\Rightarrow\; \mathbf{L}^*\left(\phi_j^*\right) = \frac{\partial \xi_j^{\text{Subspace}}}{\partial \phi}$$

Distinct Mechanism Behind the Methods

- FW-CADIS approach creates pseudo response as a linear combination of responses with weights signed to be the reverse of the corresponding responses
- Subspace approach identifies the correlations between weight window maps to minimize the computational time

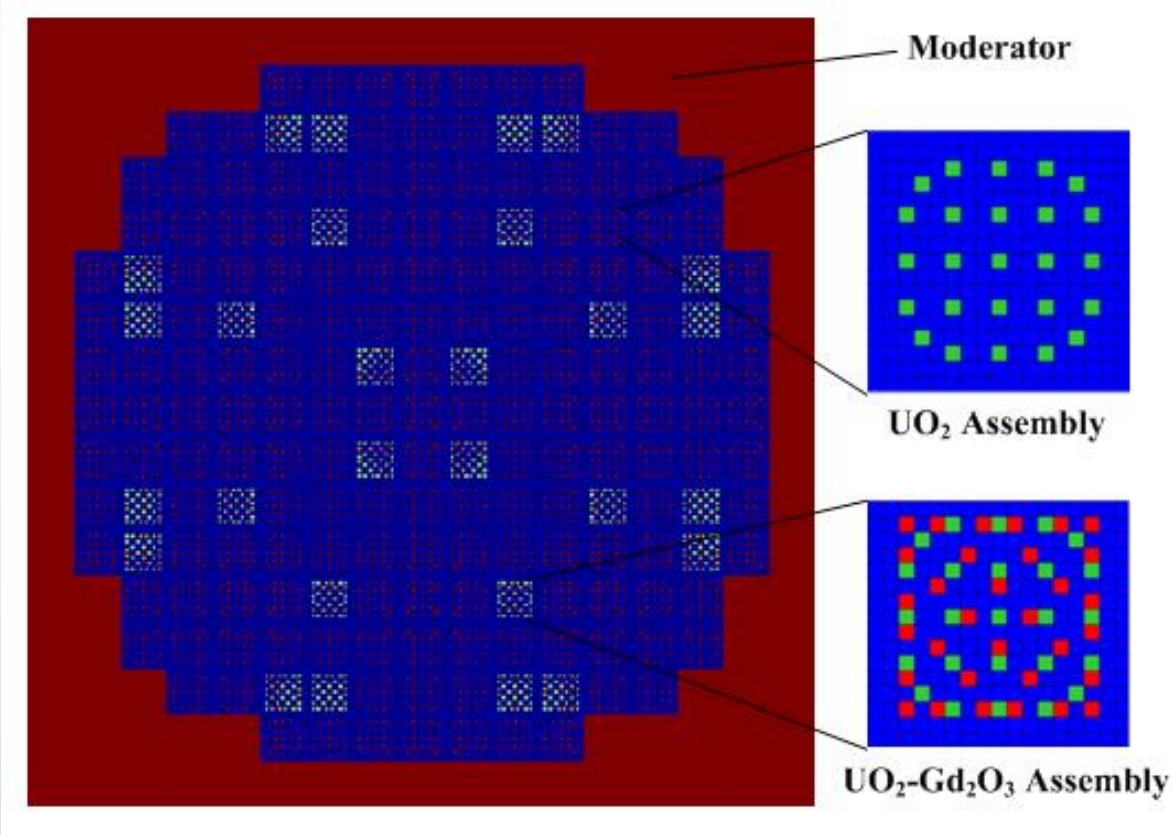
Case Study 1: BWR Assembly Model

- Code: *MAVRIC* sequences in *SCALE* package
- BWR Assembly, 7x7 array of fuel pins with various enrichments
- Fixed source subcritical system
- Total 27 neutron and 19 photon energy group library are applied



m = 49.

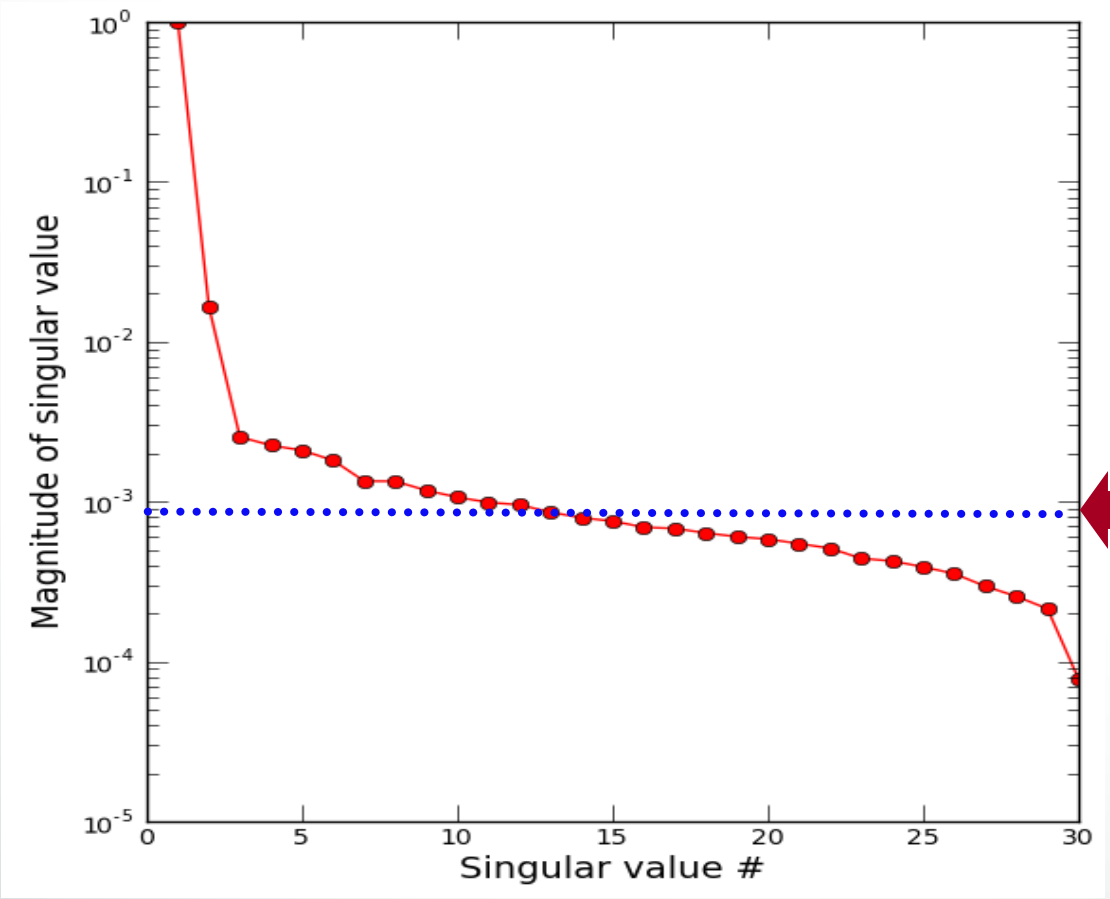
Case Study 2: PWR Core Model



m = 193.

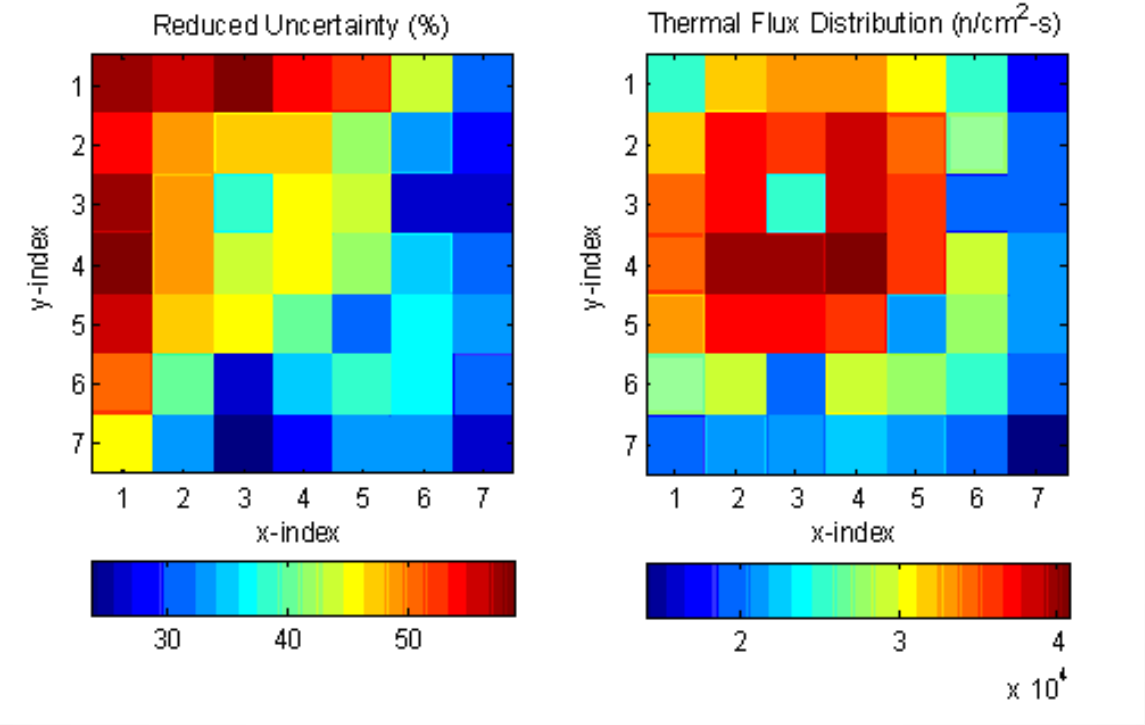
- X-Y view of the core loading pattern with details assembly described on the side
- Total 193 fuel assemblies (blue region) laid out a 17x17 grid scheme and surrounded by light water (red region)
- Two types of fuel assemblies are designed: UO_2 fuel assembly and a UO_2-Gd_2O_3 fuel assembly.

Singular Values Plot of the SRI Matrix (Assembly Model)



r = 12.

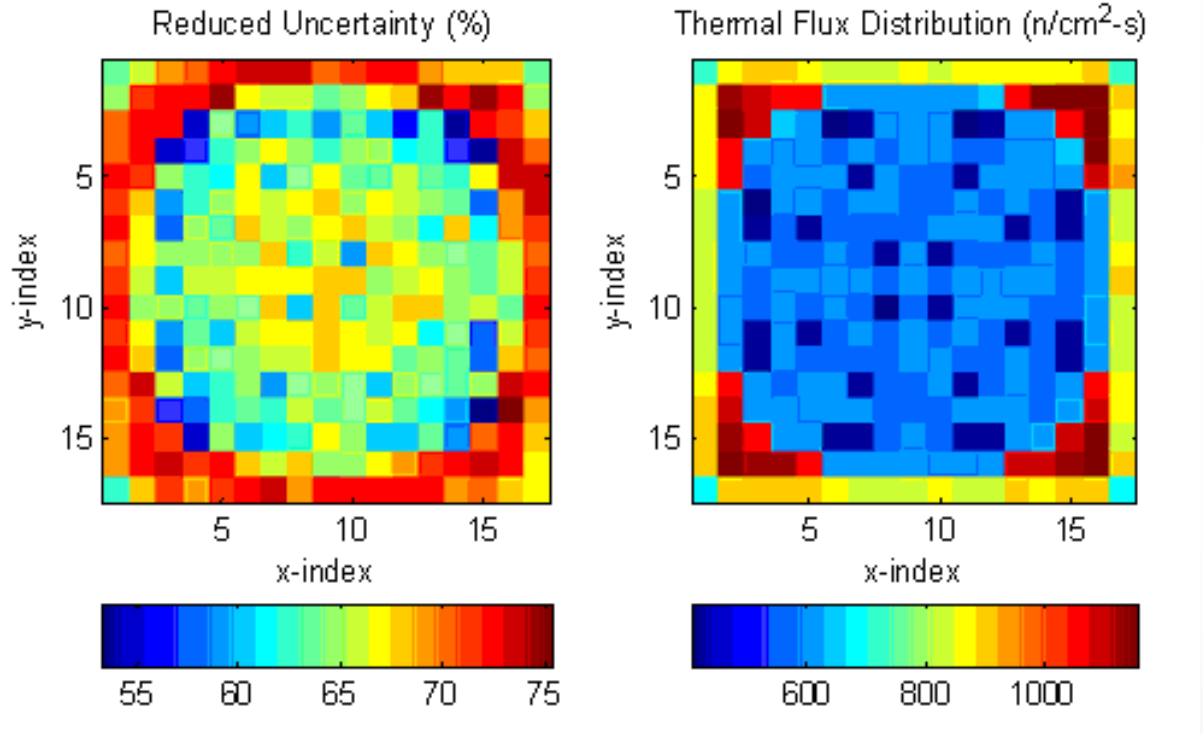
Relative Uncertainty Comparison for Thermal Flux (Subspace vs. FW-CADIS, Assembly Model)



a. Standard Deviation Reduction b. Mean Thermal Flux Distribution

$$\Delta\sigma_i = \frac{\sigma_i^{\text{FW-CADIS}} - \sigma_i^{\text{Subspace}}}{\sigma_i^{\text{FW-CADIS}}} \times 100\%$$

Relative Uncertainty Comparison for Thermal Flux (Subspace vs. FW-CADIS. Core Model)



a. Standard Deviation Reduction b. Mean Thermal Flux Distribution

$$\Delta\sigma_i = \frac{\sigma_i^{\text{FW-CADIS}} - \sigma_i^{\text{Subspace}}}{\sigma_i^{\text{FW-CADIS}}} \times 100\%$$

Conclusions for Hybrid Approaches

- Number of independent correlations are much smaller than number of responses, when responses are required everywhere in phase space
- Subspace approach takes advantage of correlations between response importance maps and employs deterministic method to identify correlations
- Subspace approach successfully gain better convergence for MC simulation comparing to FW-CADIS approach
- Idea could be extended to other hybrid deterministic-MC techniques

Sensitivity Analysis in Monte Carlo Models with GPT-Free Method

Introduction for GPT-Free Method

- **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: 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

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

General Response Sensitivity Profiles

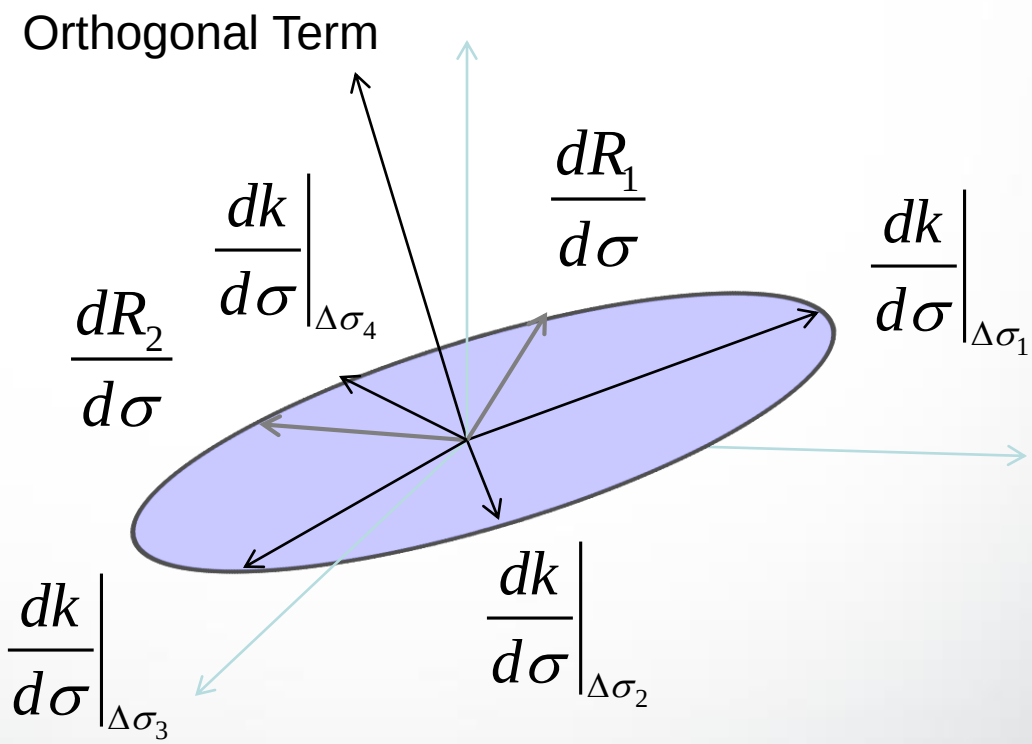
Constructing Equivalent Subspace

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

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

Subspace:

$$\text{span}\left\{ \left.\frac{dk}{d\sigma}\right|_{\Delta\sigma_i} \right\}$$

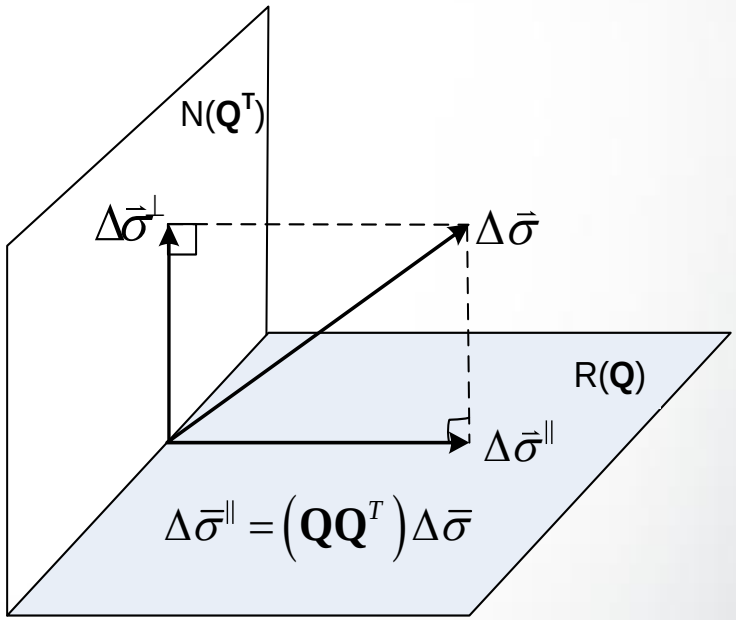


Project Parameter Perturbation onto Sensitivity Subspace

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

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



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

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,

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

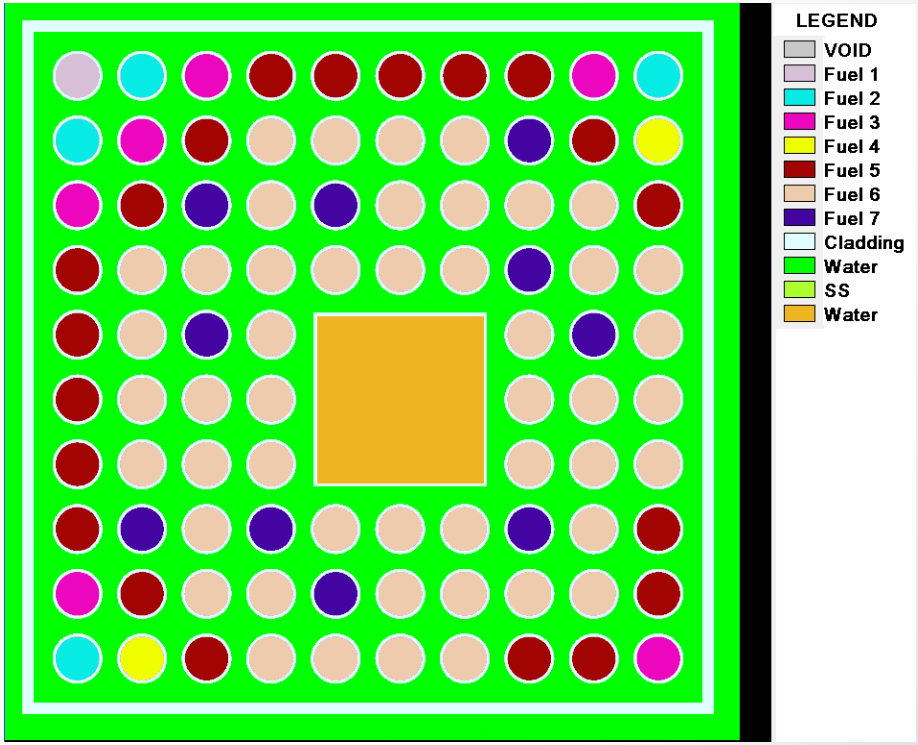
$$=f\left(\vec{\sigma}_0+\sum_{i=1}^{r}\alpha_i\vec{q}_i\right)\overset{\text{if linear}}{=}f\left(\vec{\sigma}_0\right)+\sum_{i=1}^{r}\alpha_i\left[f\left(\vec{\sigma}_0+\vec{q}_i\right)-f\left(\vec{\sigma}_0\right)\right]$$

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

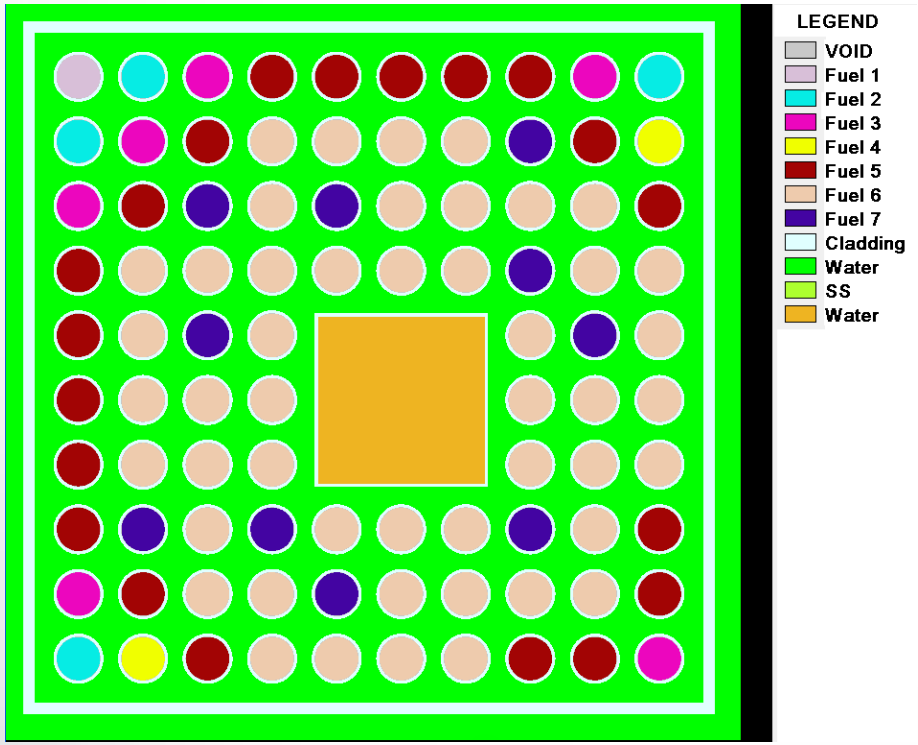
r << n !!!

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 $dk/d\bar{\sigma}\big|_i$
- Repeat *r* times and form the decomposition:

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

- 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:

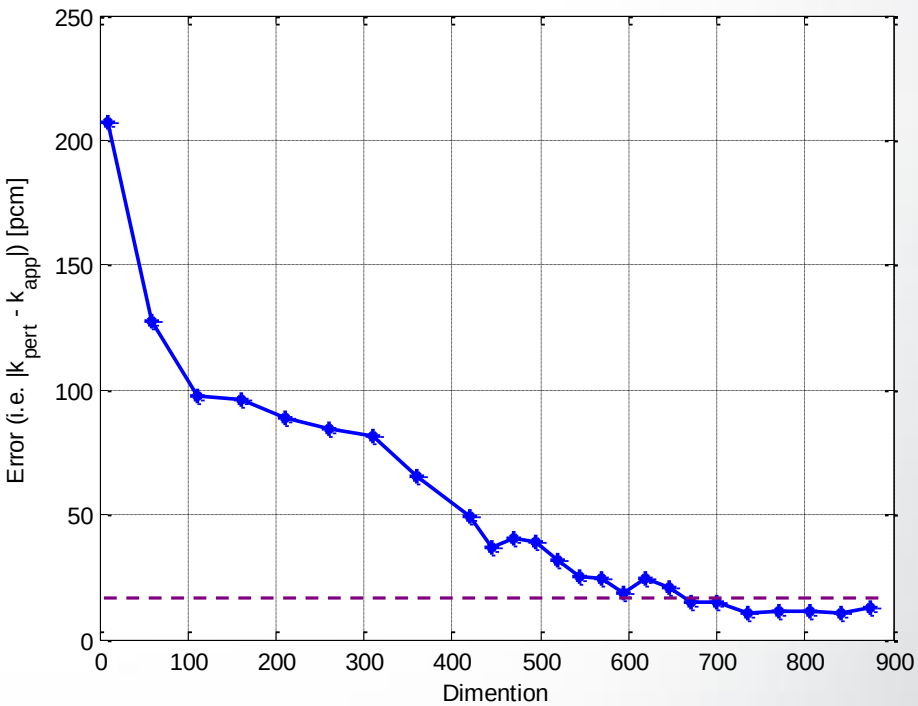
$$\kappa = \left| k_{\text{pert}} - k_{\text{app}} \right|$$

Where,

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

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

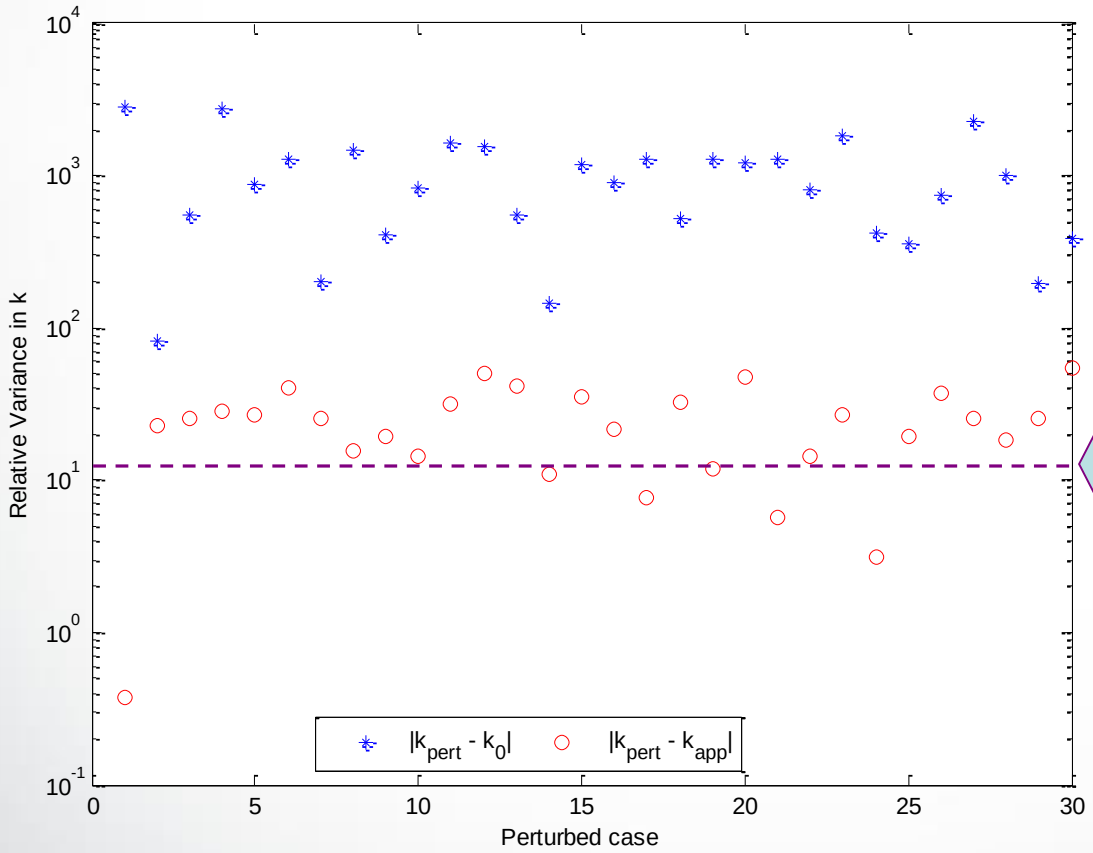
$$= k\left[\vec{\sigma}_0 + \left(\mathbf{Q}_r \boxed{\mathbf{Q}_r^T}\right)\Delta\vec{\sigma}\right]$$



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

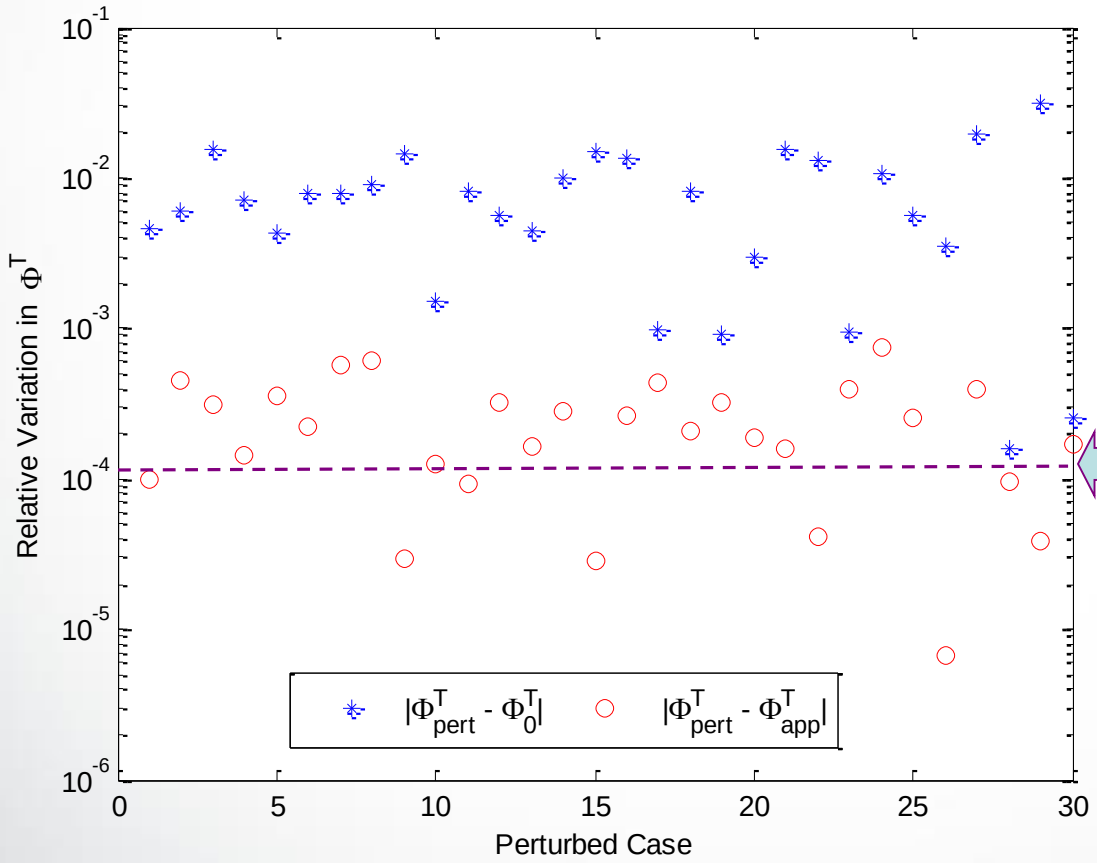
Recall ***n* = 68306**, so ***r* << *n***.

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 for GPT-Free Method

- 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.
- 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.

Summary of this Talk

- Neutronics calculations and uncertainty quantification in modeling and simulation of nuclear reactor are briefly introduced, the outstanding challenges and standard methods associated with them are addressed
- Two interesting researches related to reactor physics calculations are presented, and they both can be casted as advanced techniques in modeling and simulation (M&S) in neutronics analysis area
- Difficulties existing in current work are discussed, and some possible research directions for future exploration are also recommended