Advanced Research Activities in Nuclear Engineering

Zeyun Wu, Ph.D.

Department of Nuclear Engineering
North Carolina State University

Fusion Science and Technology Center
University of California, Los Angeles

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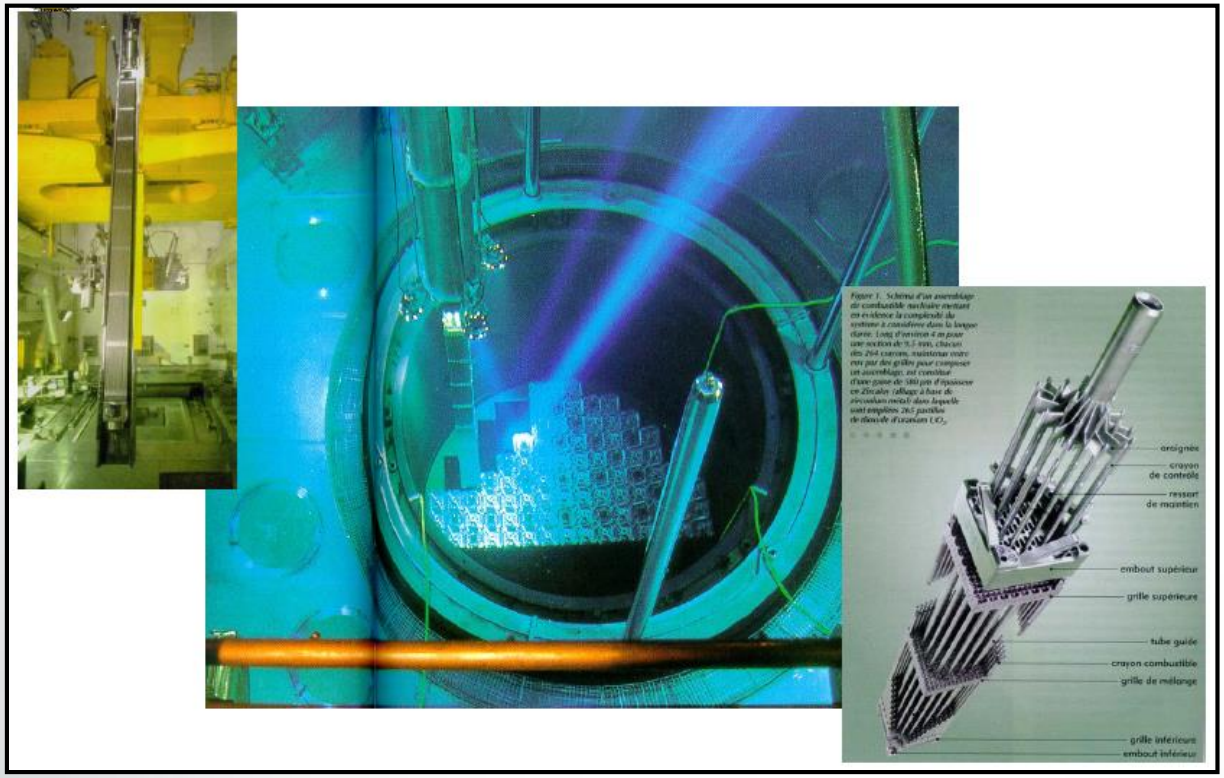
Overview of Neutronics

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)

Challenges in Neutronics Analysis

- 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
  - Complexity in nuclide cross sections
  - Multi-physics coupling problem
  - Nuclear data sensitivities and uncertainties

Neutronics Analysis Approaches

- Deterministic method
  - Transport process is described by integro-differential Boltzmann equation with specified boundary conditions
  - Major codes: NEWT, DENOVO, ATTILA, PARTISN, CASMO, SIMULATE, DeCART, etc.
- Monte Carlo method
  - Radiation transport is inherently linked to physics by simulating random history of individual particles.
  - Major codes: MCNP, EGS, GEANT, KENO, MONACO, etc.

Sensitivity Analysis in Monte Carlo Models with GPT-Free Method

(Co-worked with Ph.D. student Chris Ken and Dr. Hany Abdel-Khalik.)

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: 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

$$k = f(\phi)$$

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

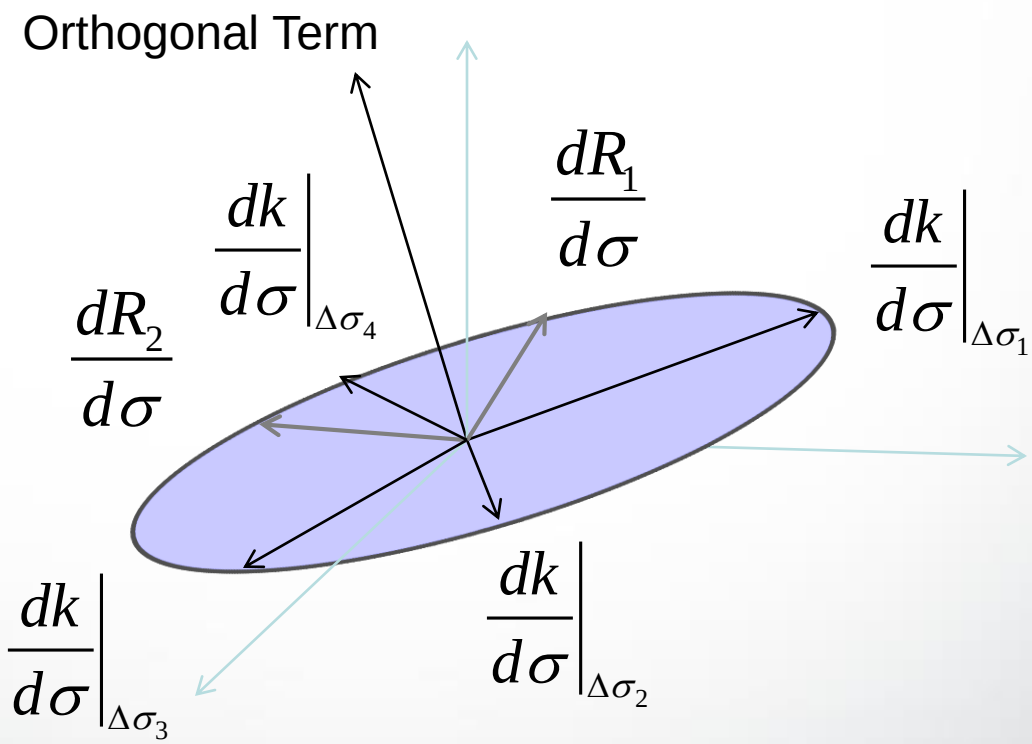
Constructing Equivalent Subspace

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:

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

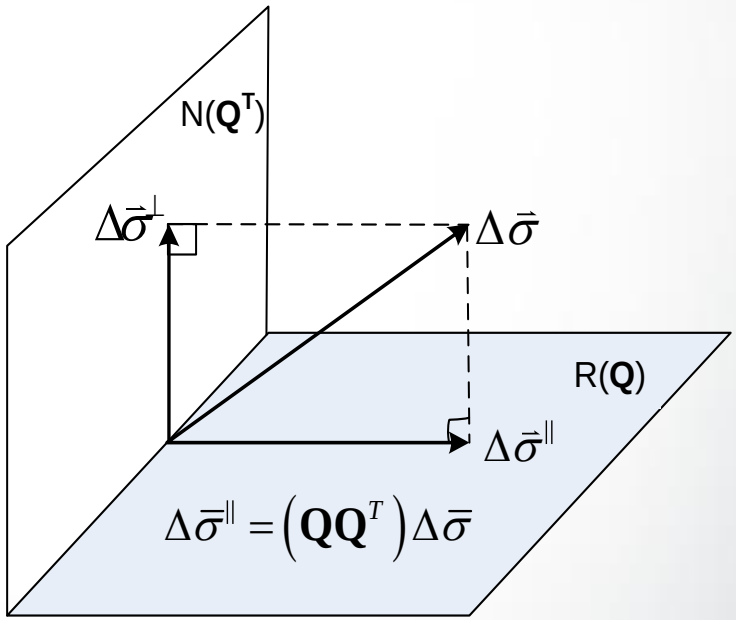


Project Parameter Perturbation onto Sensitivity Subspace

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,

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

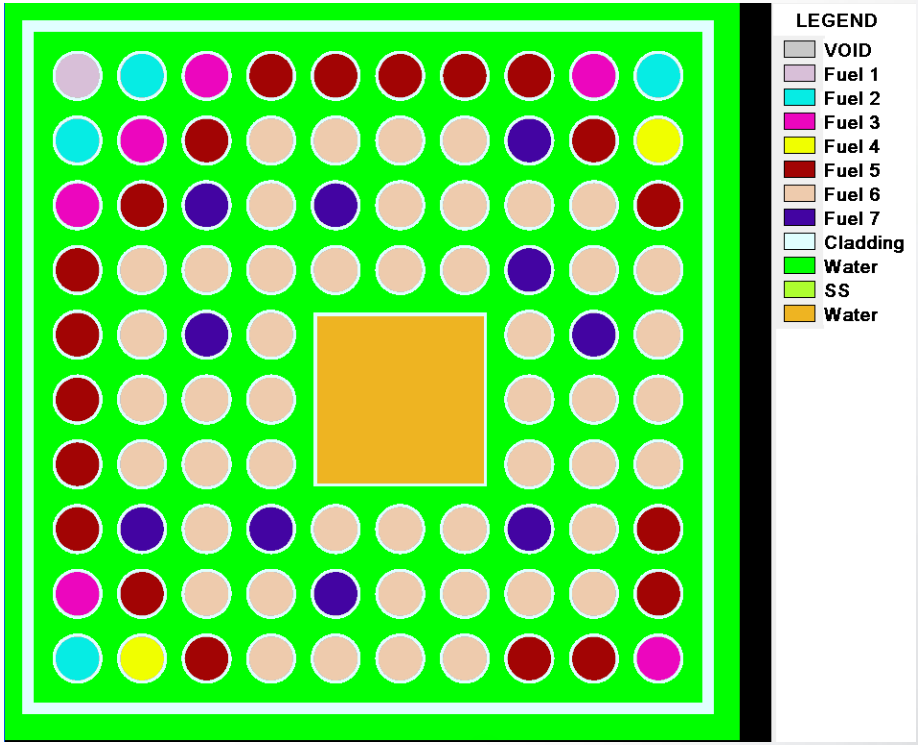
$$=f\left(\vec{\sigma}_0+\sum_{i=1}^{r}\alpha_i\vec{q}_i\right)\overset{\text{if linear}}{=}f\left(\vec{\sigma}_0\right)+\sum_{i=1}^{r}\alpha_i\left[f\left(\vec{\sigma}_0+\vec{q}_i\right)-f\left(\vec{\sigma}_0\right)\right]$$

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

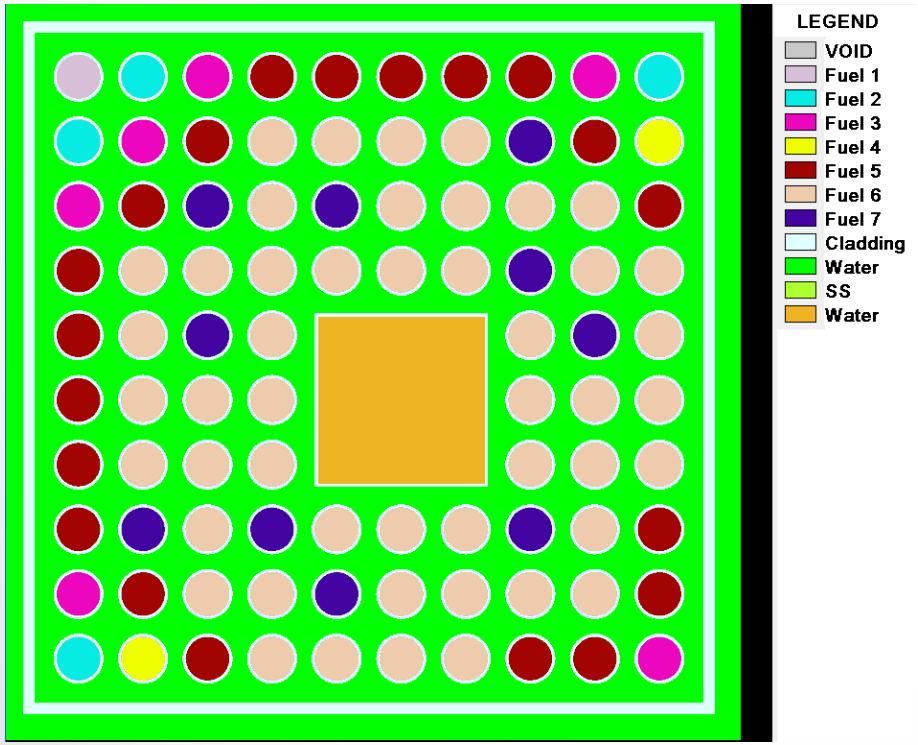
r << n !!!

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:

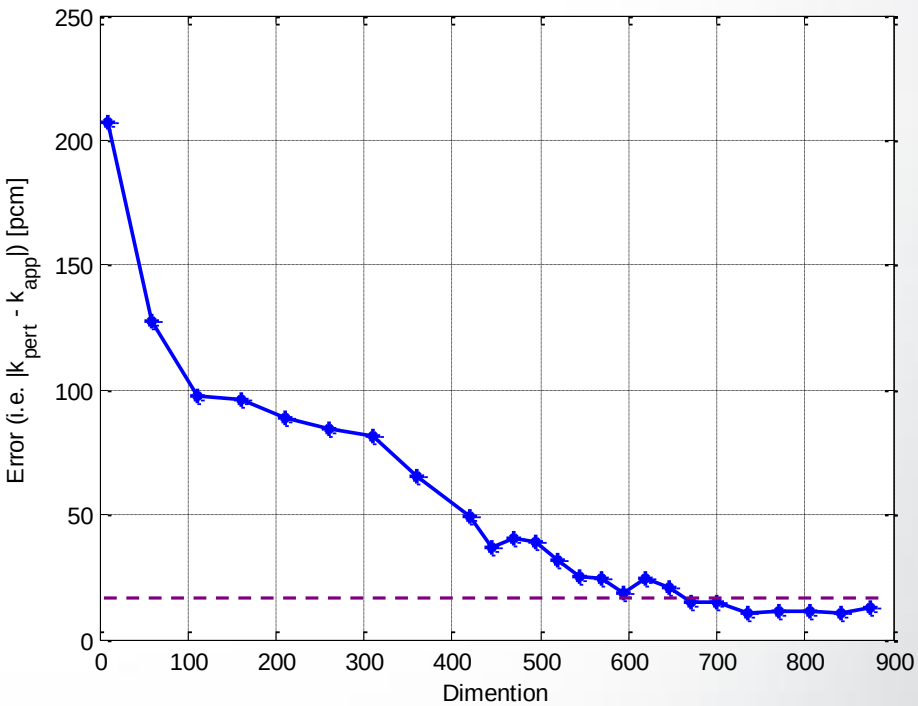
$$\kappa = \left| k_{\text{pert}} - k_{\text{app}} \right|$$

Where,

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

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

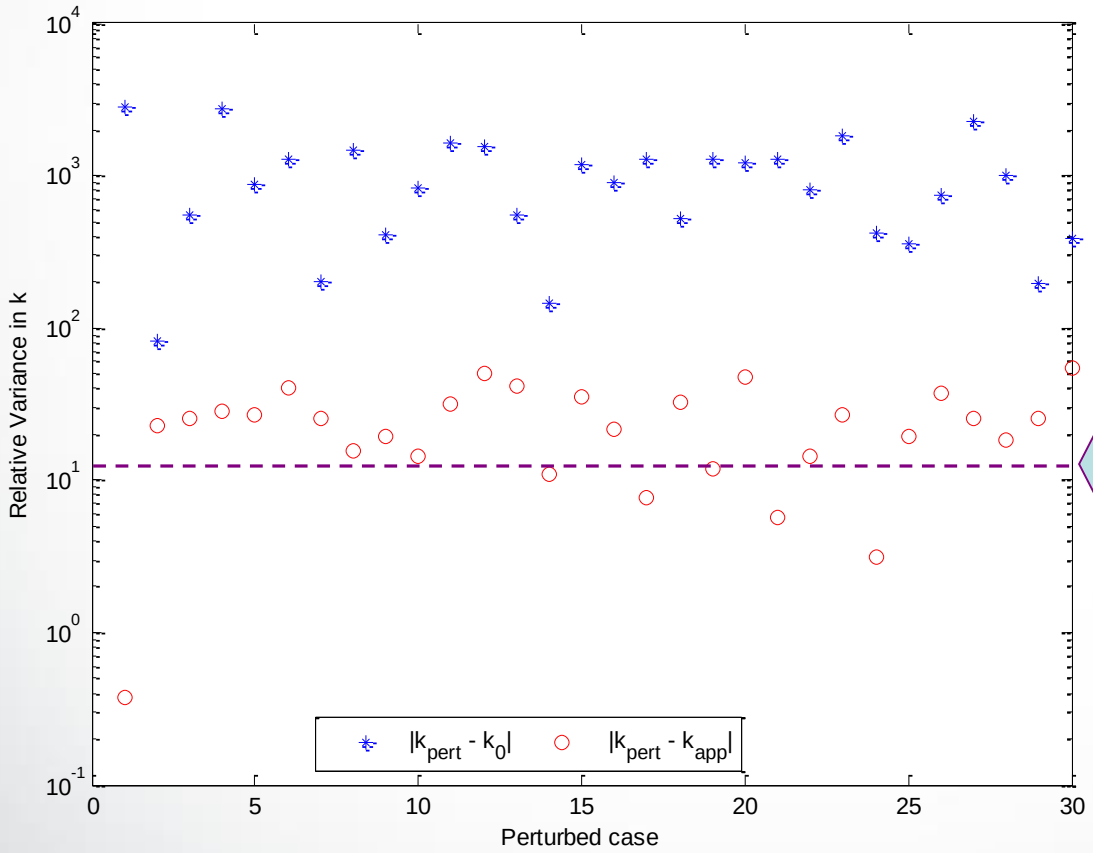
$$= k\left[\vec{\sigma}_0 + \left(\mathbf{Q}_r \boxed{\mathbf{Q}_r^T}\right)\Delta\vec{\sigma}\right]$$



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

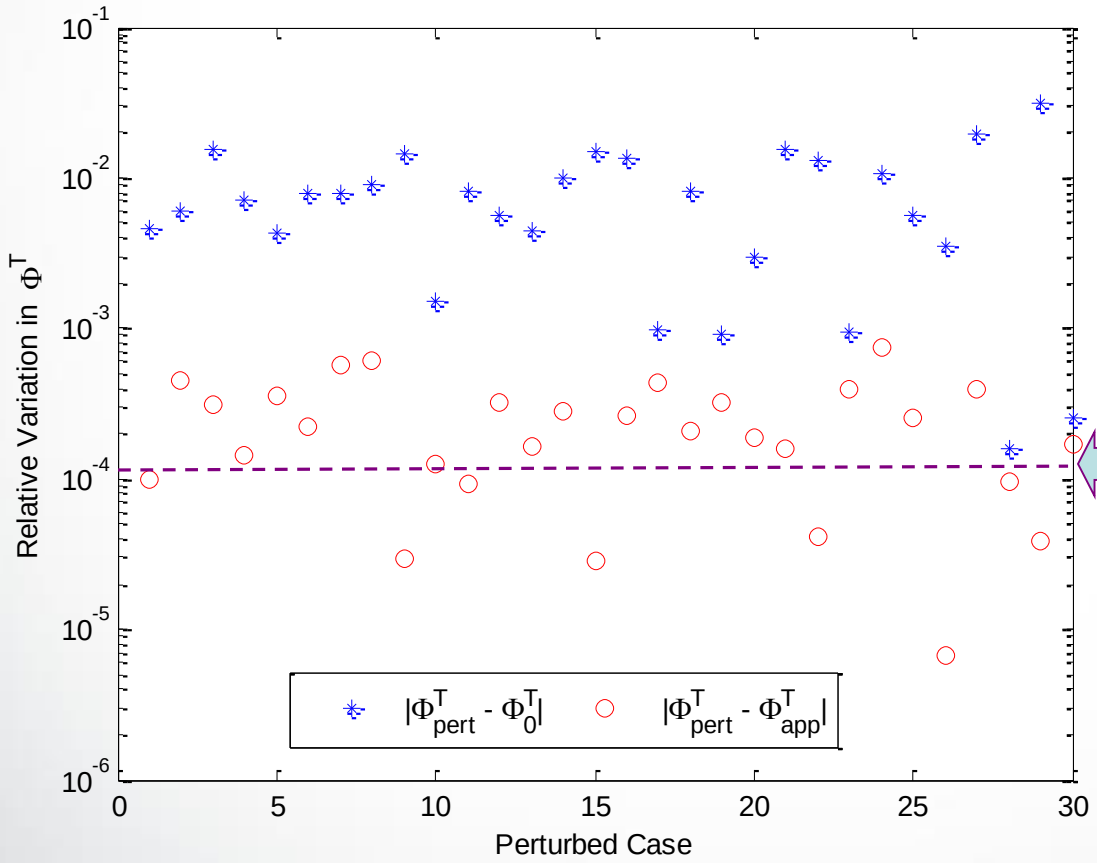
Recall ***n* = 68306**, so ***r* << *n***.

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.

Hybrid Monte Carlo – Deterministic Transport Approaches

(Co-worked with Ph.D. student Qiong Zhang and Dr. Hany Abdel-Khalik.)

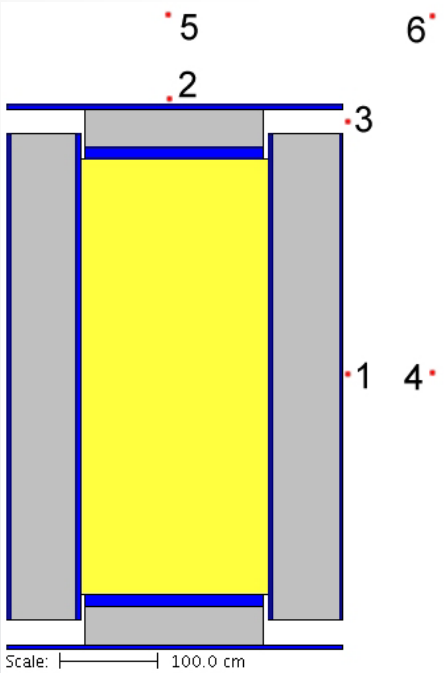
Introduction for Hybrid Approach

- 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)

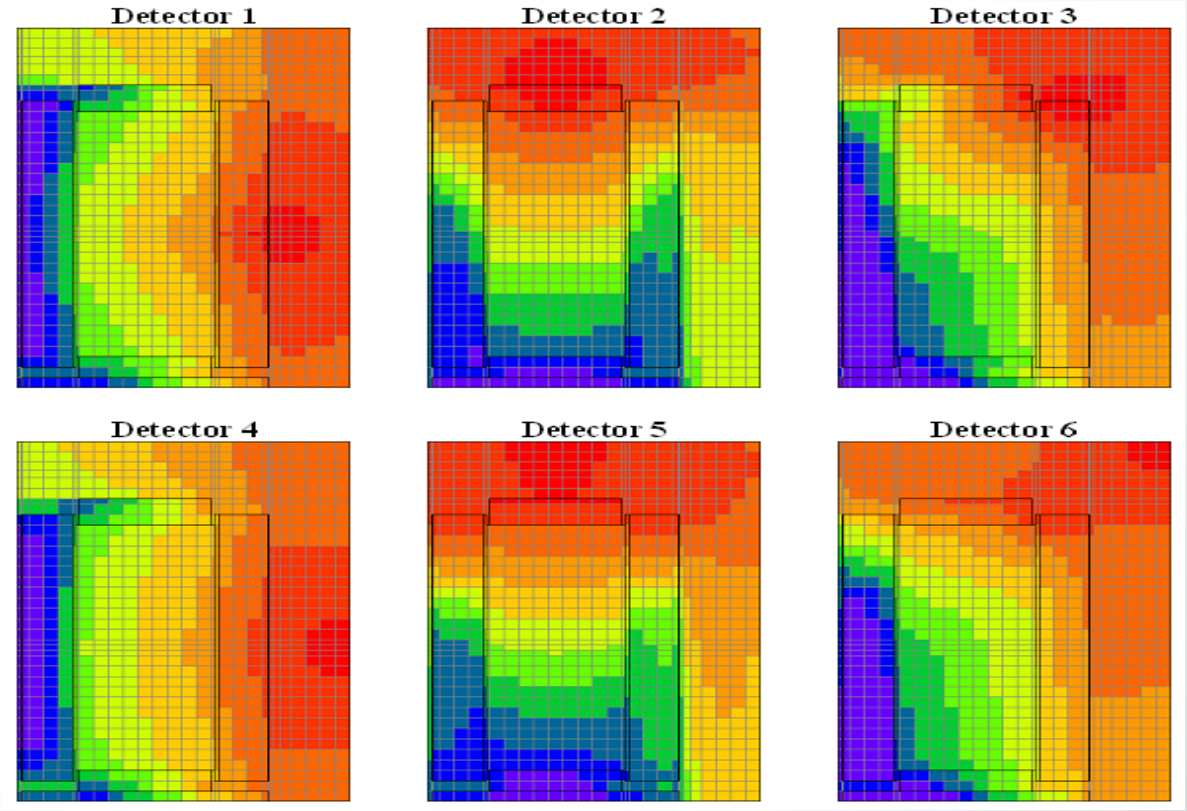
Current Challenges in Hybrid Approaches

- 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



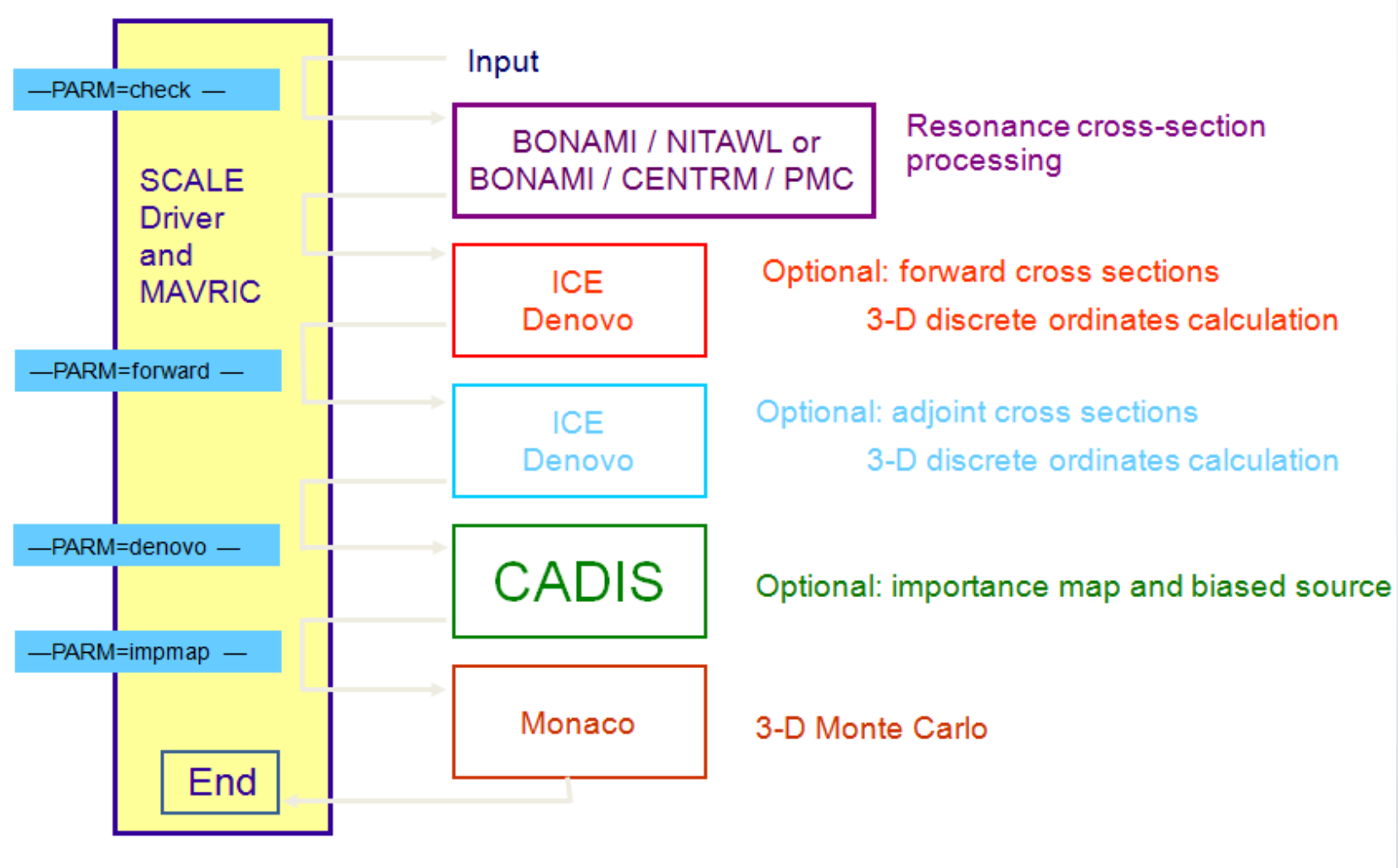
Corresponding Adjoint Flux Profiles

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

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

FW-CADIS MAVRIC Sequence in SCALE



Our Proposed Approaches

- 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
- Two variant approaches based on these ideas are proposed
  - **Subspace** approach
  - **Gaussian Process (GP)** Approach

Correlations?

- Given *m* random variables: $X_1, \ldots, X_m$
- Correlations are described by:

$$\operatorname{cov}\left(X_i, X_j\right) = \mathrm{E}\left[\left(X_i - X_i^{\mu}\right)\left(X_j - X_j^{\mu}\right)\right] = C_{i,j}$$

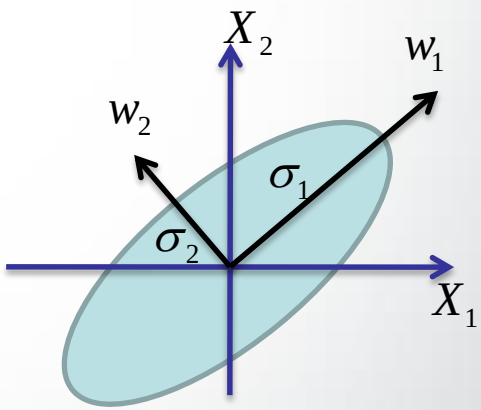
$$\mathbf{C} = \mathbf{W}\boldsymbol{\Sigma}^2\mathbf{W}^T \approx \mathbf{W}_r\boldsymbol{\Sigma}_r^2\mathbf{W}_r^T$$

$$\rightarrow \mathbf{W} = \begin{bmatrix} w_1 & \ldots & w_m \end{bmatrix} \in \mathbf{R}^{m\times m}$$

$$\rightarrow \boldsymbol{\Sigma} = \operatorname{diag}\left\{\sigma_1, \ldots, \sigma_m\right\} \in \mathbf{R}^{m\times m}$$

$$\rightarrow \mathbf{W}_r = \begin{bmatrix} w_1 & \ldots & w_r \end{bmatrix} \in \mathbf{R}^{m\times r}$$

$$\rightarrow \boldsymbol{\Sigma}_r = \operatorname{diag}\left\{\sigma_1, \ldots, \sigma_r\right\} \in \mathbf{R}^{r\times r}$$



Subspace Approach

- Identifies the correlations between weight window maps to minimize the computational time
- *r* pseudo response are formed 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)
- Final solutions (mean and variance values) are estimated as follows

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

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

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

Gaussian Process (GP) Approach

- Radiation transport may be treated as a Gaussian Process
- If responses correlations (covariance matrix) can be estimated, one can reduce it to identify *r* uncorrelated pseudo responses
- *r* pseudo responses are formed in **GP** approach

$$\xi_j^{\mathrm{GP}} = \sum_{i=1}^{m} w_{i,j} r_i, \quad j = 1, \ldots, r$$

GP Approach - Estimating Responses Covariance Matrix

Let $\vec{r} = \begin{bmatrix} r_1 & r_2 & \dots & r_m \end{bmatrix}^T \in \mathbf{R}^m$ represent a vector of the *m* responses of interest representing *m* random Gaussian processes. Denote $\left\{ r_i^k \right\}_{i=1}^m, k = 1, 2, \dots, N$ as *N* realizations of these random processes. The covariance between the two responses r_i and r_j is given by:

$$\operatorname{cov}(r_i, r_j) = \lim_{N \to \infty} \frac{1}{N-1} \sum_{k=1}^{N} \left(r_i^k - \hat{r}_i \right) \left(r_j^k - \hat{r}_j \right)$$

The covariance information between all pairs of *m* responses may also be represented by a symmetric covariance matrix $\mathbf{C} \in \mathbf{R}^{m \times m}$ such that: $\mathbf{C}_{ij} = \operatorname{cov}(r_i, r_j)$. The SVD form of this matrix is:

$$\mathbf{C} = \mathbf{W} \boldsymbol{\Sigma} \mathbf{W}^T = \sum_{i=1}^{m} \sigma_i \vec{w}_i \vec{w}_i^T \approx \sum_{i=1}^{r} \sigma_i \vec{w}_i \vec{w}_i^T$$

Summary of Importance-based Biasing Approaches

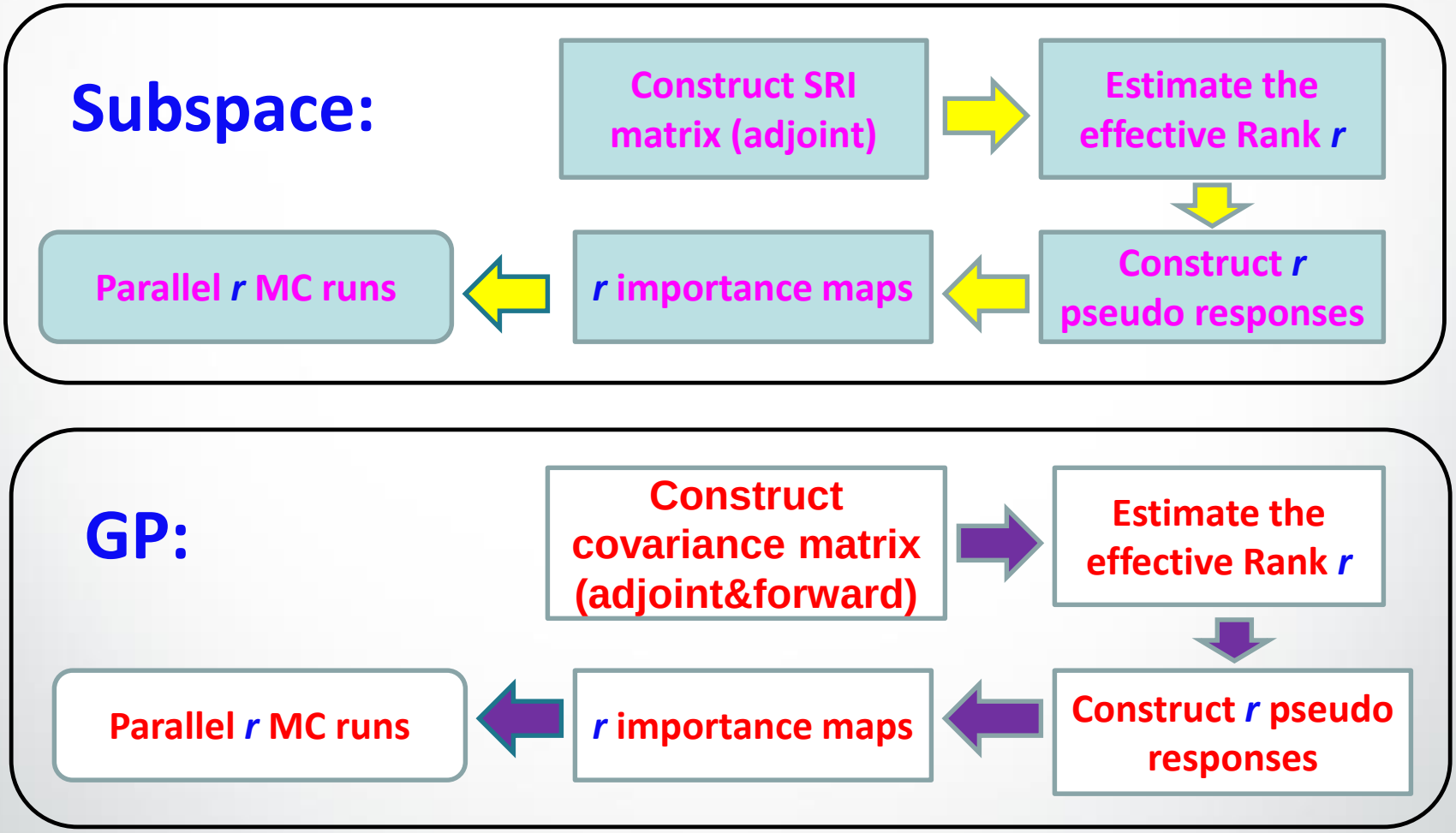
- Deterministic Model: $\mathbf{L}^*\left(\phi_i^*\right) = \dfrac{\partial r_i}{\partial \phi}$
- FW-CADIS: $\mathbf{L}^*\left(\phi^*\right) = \dfrac{\partial \xi}{\partial \phi} \rightarrow \xi^{\text{FW-CADIS}} = \sum_{i=1}^{m} r_i / \phi_i$
- Subspace Approach: $\xi_j^{\text{Subspace}} = \sum_{i=1}^{m} \alpha_{i,j} r_i, \quad j = 1, \ldots, r$
- GP Approach: Find covariance matrix, identify *r* pseudo responses

$$\xi_j^{\text{GP}} = \sum_{i=1}^{m} w_{i,j} r_i, \quad j = 1, \ldots, r$$

Distinct Mechanism Behind Three Methods

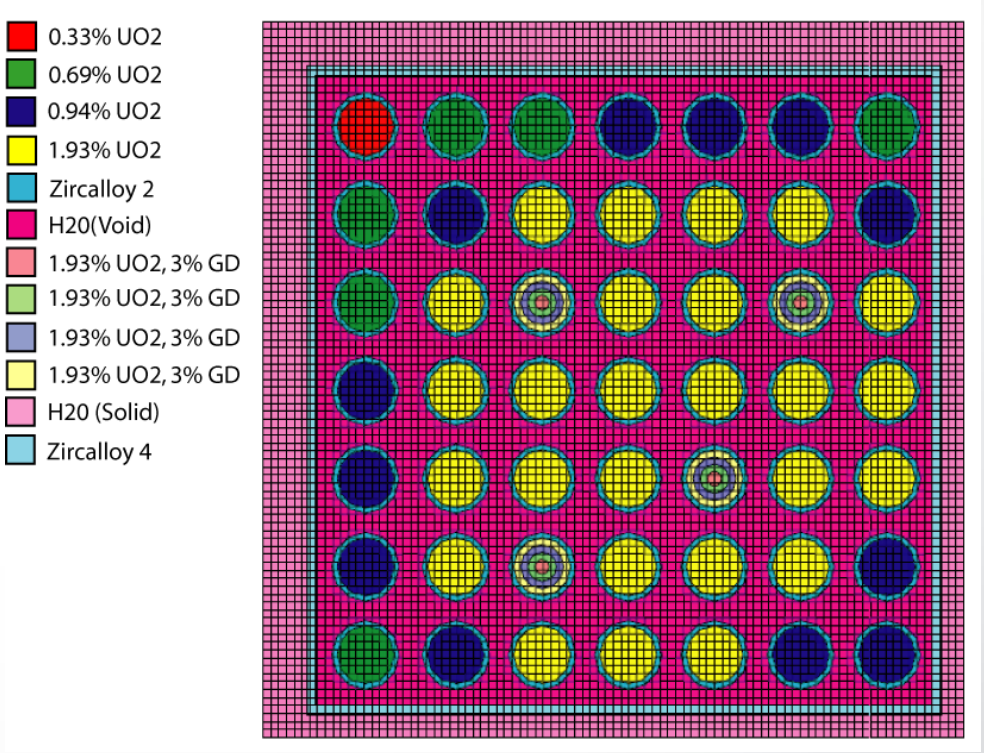
- FW-CADIS creates pseudo response as a linear combination of responses with weights signed to be the reverse of the corresponding responses
- Subspace approach identifies the correlations between weight window maps to minimize the computational time
- GP approach formulates pseudo responses based on the effective rank of the covariance matrix to the responses of interest

Algorithm Flowchart for Proposed Approaches

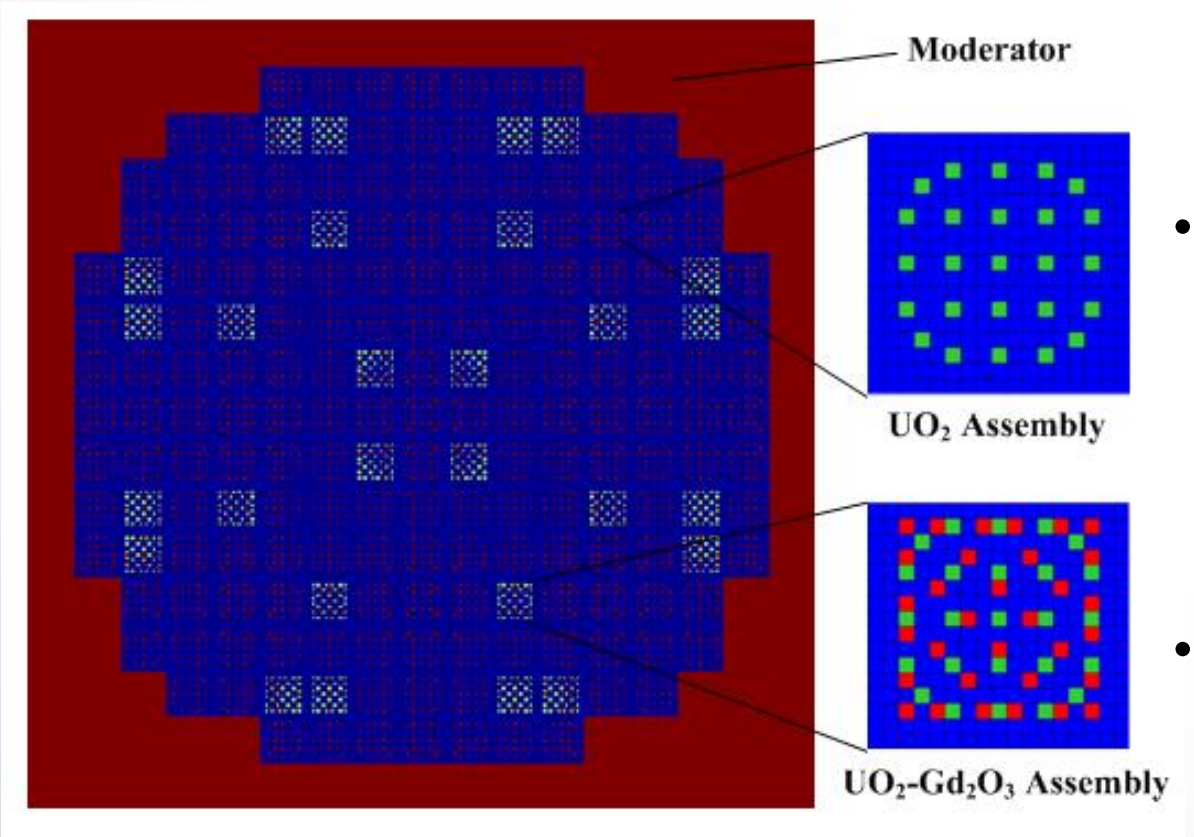


Case Study 1: BWR Assembly Model

- 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

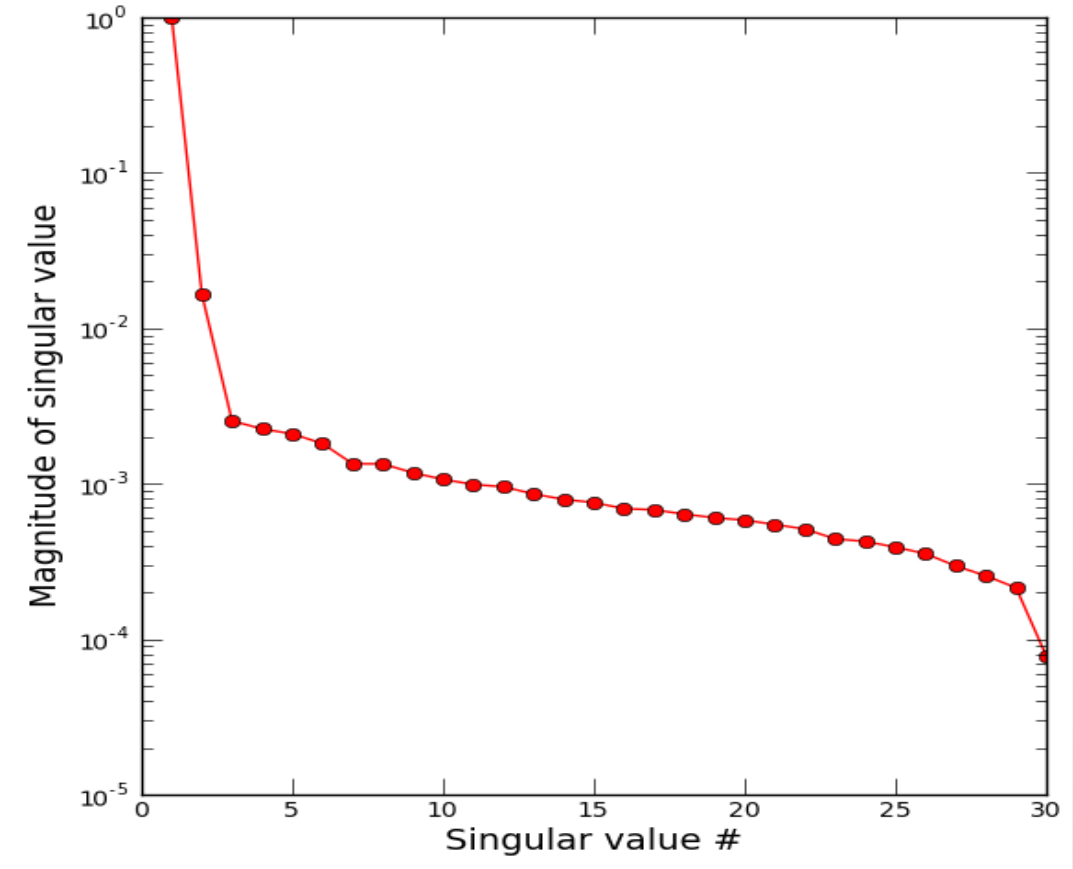


Case Study 2: PWR Core Model

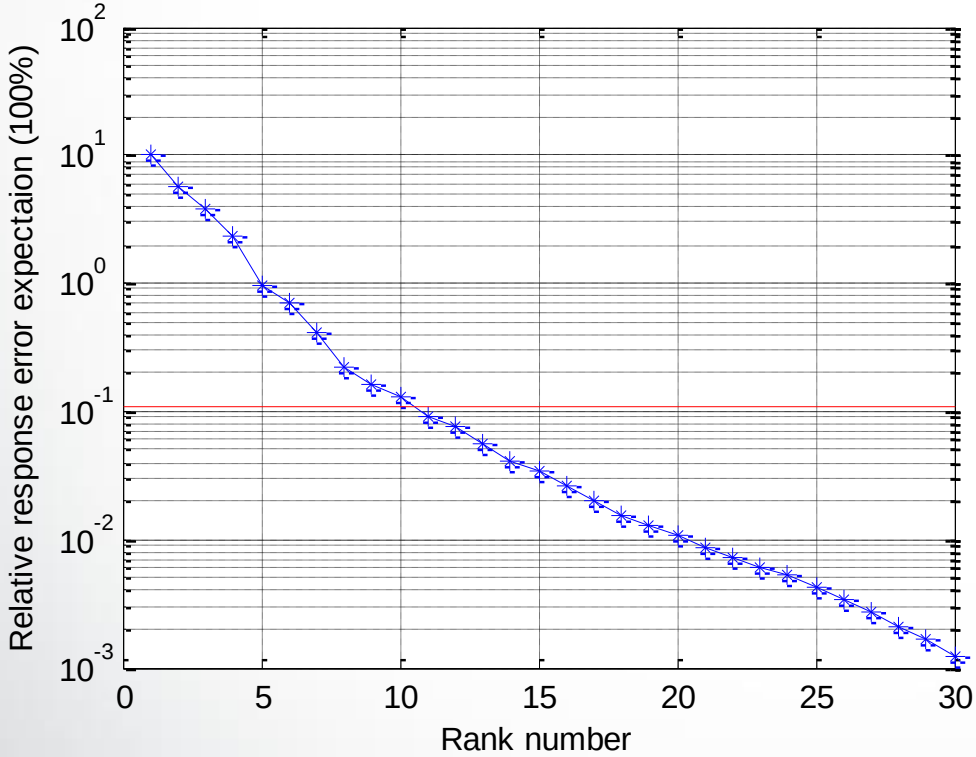


- X-Y view of the core loading pattern with details assembly described on the side
- Total 193 fuel assemblies (blue region) laid out a 17x17 grid scheme and surrounded by light water (red region)
- Two types of fuel assemblies are designed: UO_2 fuel assembly and a UO_2-Gd_2O_3 fuel assembly.

Singular Values of the SRI Matrix (Subspace Approach)



Estimate of the Effective Rank for Covariance Matrix (GP Approach)



SVD of Covariance Matrix:

$$\mathbf{C} = \mathbf{W}\boldsymbol{\Sigma}^2\mathbf{W}^T = \sum_{i=1}^{m} \sigma_i^2 \vec{w}_i \vec{w}_i^T$$

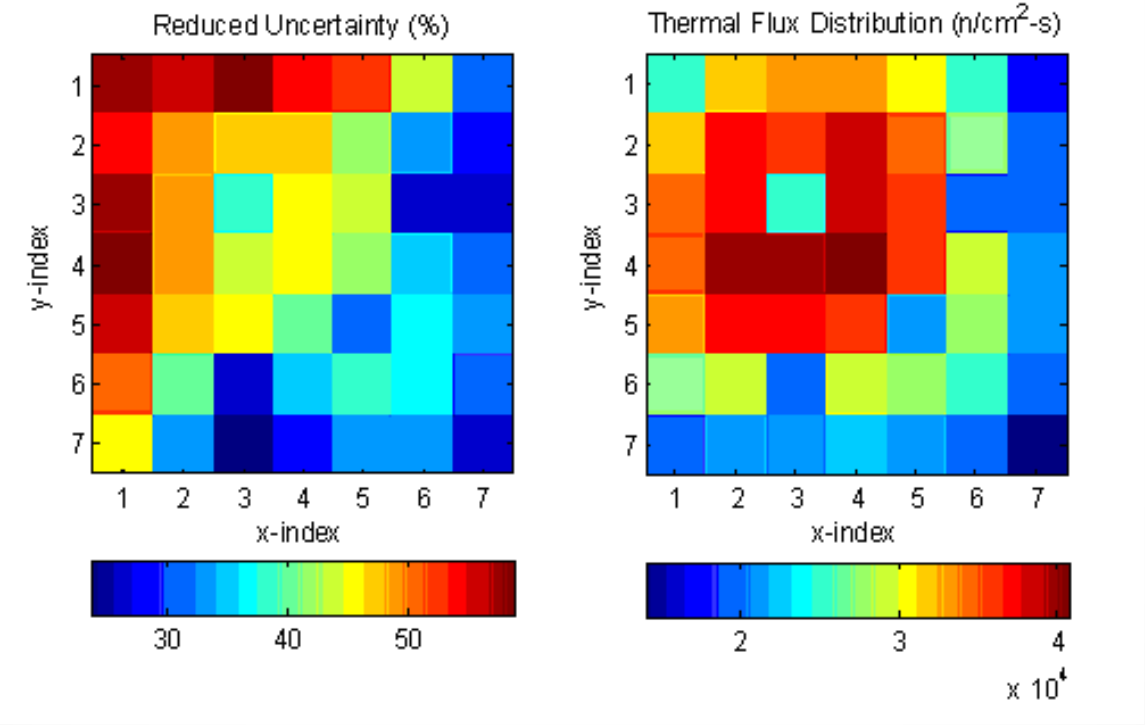
Truncated SVD Approximation:

$$\mathbf{C}_r = \sum_{i=1}^{r} \sigma_i^2 \vec{w}_i \vec{w}_i^T$$

Search Criterion:

$$\left\| \mathbf{C} - \mathbf{C}_r \right\| < \delta$$

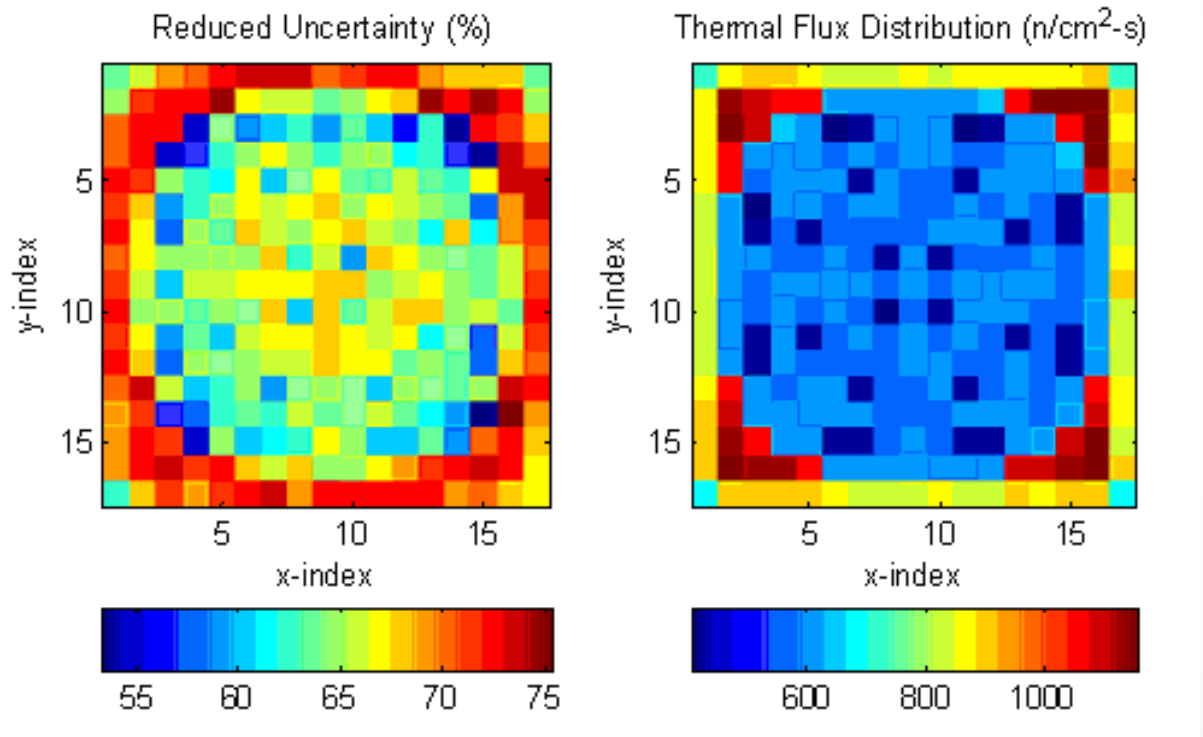
Relative Uncertainty Comparison for Thermal Flux (Subspace vs. FW-CADIS, Assembly Model)



a. Standard Deviation Reduction b. Mean Thermal Flux Distribution

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

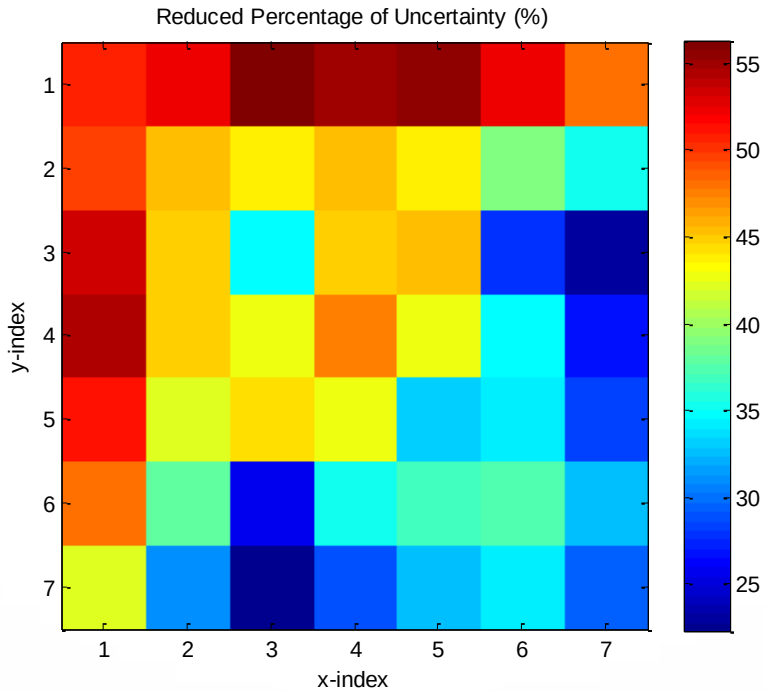
Relative Uncertainty Comparison for Thermal Flux (Subspace vs. FW-CADIS, Core Model)



a. Standard Deviation Reduction b. Mean Thermal Flux Distribution

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

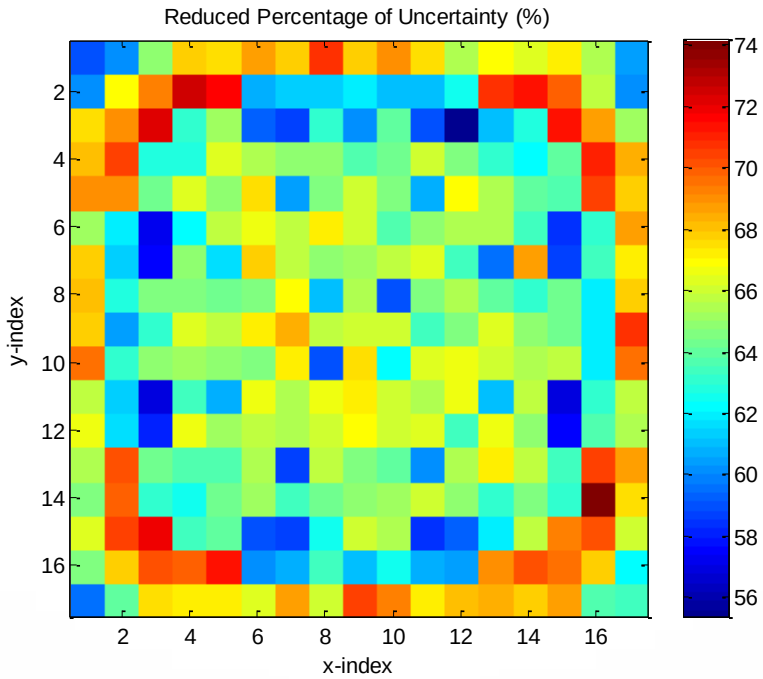
Relative Uncertainty Comparison for Thermal Flux (GP vs. FW-CADIS, Assembly Model)



Standard Deviation Reduction For Assembly Level Thermal Flux Tally

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

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



Standard Deviation Reduction For Assembly Level Thermal Flux Tally

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

Conclusions for Hybrid Approaches

- Number of independent correlations are much smaller than number of responses, when responses are required everywhere in phase space
- Both Subspace and GP provides one approach to take advantage of responses uncertainties correlations and deterministic models can be employed to identify correlations
- Both Subspace and GP approach successfully gain better convergence for MC simulation comparing to FW-CADIS approach
- Comparatively, Subspace approach has closer performance to GP approach
- Idea could be extended to other hybrid deterministic-MC techniques
- The applicability of the proposed approaches remains to be tested for eigenvalue problems

Inverse Transport Problem

(Ph.D. Research Done at Texas A&M University,

advised by Dr. Marvin Adams.)

Forward vs. Inverse

- Forward Transport Problem

$$\underline{\Omega}\bullet\underline{\nabla}\psi_g(\underline{r},\underline{\Omega})+\Sigma_{tg}(\underline{r})\psi_g(\underline{r},\underline{\Omega})=\sum_{g'=1}^{G}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\underline{\Omega})\Sigma^{l}_{sg'\to g}(\underline{r})\phi_{lm,g'}(\underline{r})+S_{ext,g}(\underline{r},\underline{\Omega})$$

- Inverse Transport Problem

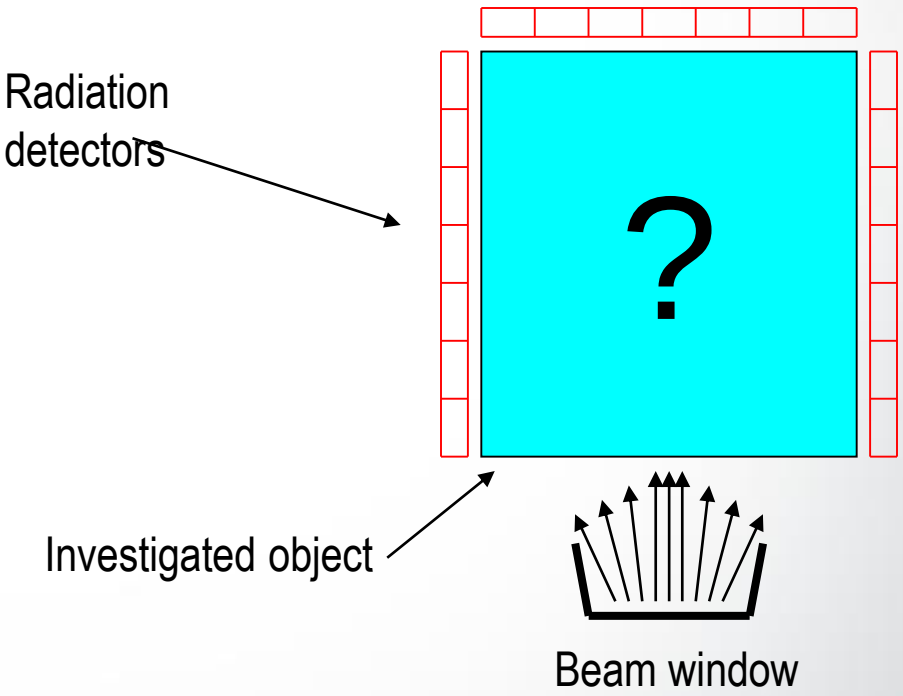
$$\underline{\Omega}\bullet\underline{\nabla}\psi_g(\underline{r},\underline{\Omega})+\Sigma_{tg}(\underline{r})\psi_g(\underline{r},\underline{\Omega})=\sum_{g'=1}^{G}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\underline{\Omega})\Sigma^{l}_{sg'\to g}(\underline{r})\phi_{lm,g'}(\underline{r})+S_{ext,g}(\underline{r},\underline{\Omega})$$

Note: Symbols in red are unknown variables in the problem.

Solve the Inverse Problem

The purpose of this research is to infer material distribution inside an object based upon detection and analysis of radiation emerging from the object.

Particular interest here is the problems in which radiation can undergo significant scattering within the object.



Model Problem

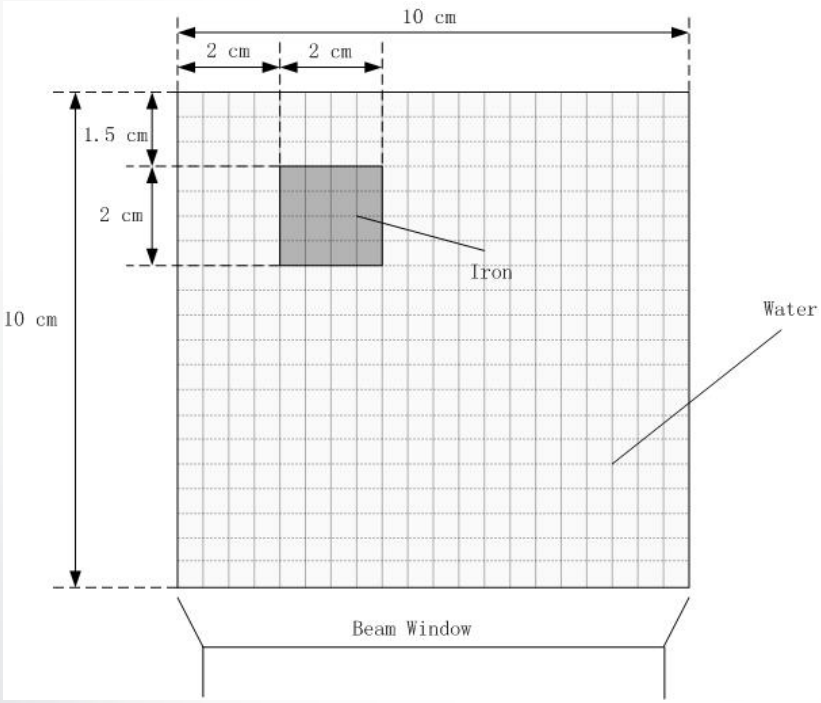


Fig: Schematic diagram of the one iron inclusion model problem (X-Y view).

Table: Physics properties of the materials in the model problem

Material	Water	Iron
Σ_s(1/cm)	0.736	0.967
Σ_t(1/cm)	0.744	1.19
g (2/3A)	3.70E-2	1.20E-2
Σ_{tr}(1/cm)	0.716	1.167
mfp(cm)	1.350	0.848
c	0.990	0.820

$$\Sigma_{tr} = \Sigma_t - g\Sigma_s, \quad mfp = \frac{1}{\Sigma_t}, \quad c = \frac{\Sigma_s}{\Sigma_t}$$

Tomographic Reconstruction Methods

- Analytic methods
  - Line integral (Radon transform)
  - Fourier slice theorem (FST)
  - Back projection reconstruction (BPR)

- Iteration methods

  forward model & inverse update scheme

  Iteration image reconstruction (IIR) methods mainly differ in their choice of forward model and how the spatial distributions of the optical properties of the medium are updated.

Analytic Methodology

- Line Integral (Radon transform)

$$P_\theta(t) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)\delta(x\cos\theta + y\sin\theta - t)dxdy$$

- Fourier Slice Theorem (FST)

$$F(u,v) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)e^{-j2\pi(ux+vy)}dxdy$$

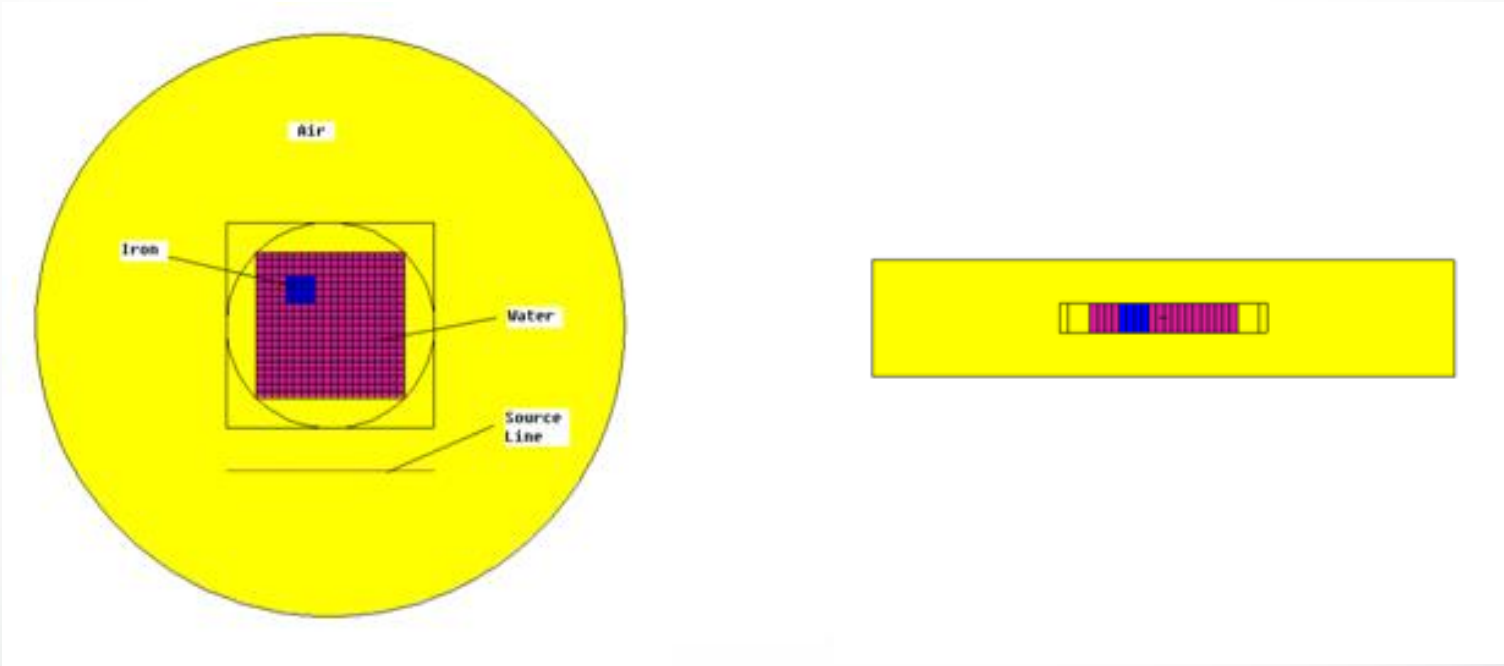
$$S_\theta(\omega) = \int_{-\infty}^{+\infty} P_\theta(t)e^{-j2\pi\omega t}dt$$

$$S_\theta(\omega) = F(\omega\cos\theta, \omega\sin\theta)$$

- Filter Back Projection (FBP)

$$f(x,y) = \int_0^{\pi}\left[\int_{-\infty}^{+\infty} S_\theta(\omega)|\omega|e^{j2\pi\omega t}d\omega\right]d\theta$$

MCNP Modeling to Provide Projections



(a) X-Y View (b) X-Z View

Fig: Test problem layout and experimental configuration

Multiple Groups of Projections

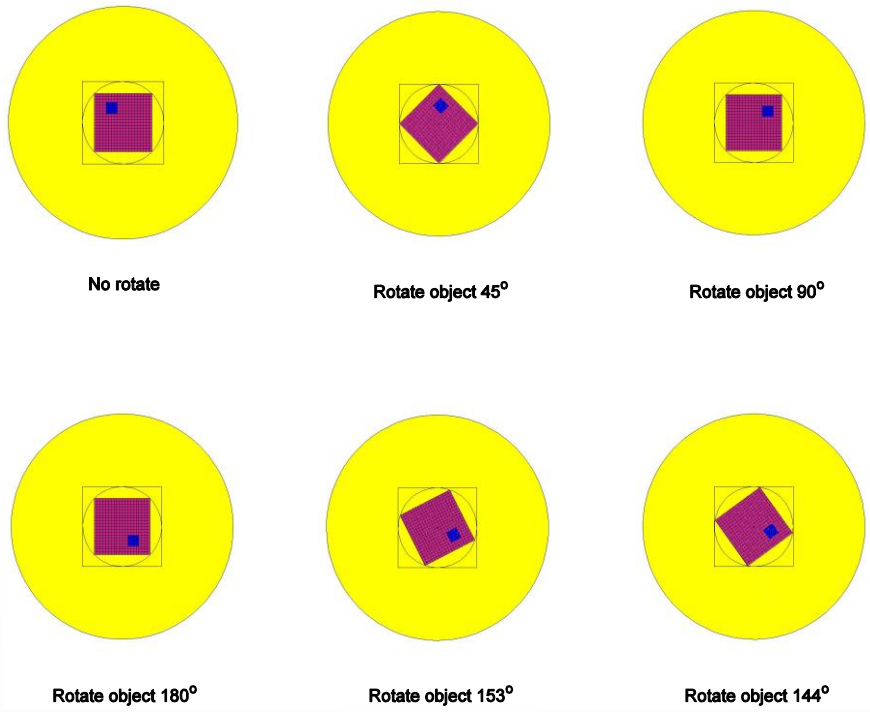


Fig: Rotate the object in different angles using mcnp_pstudy.

Plots of Radiation Projections

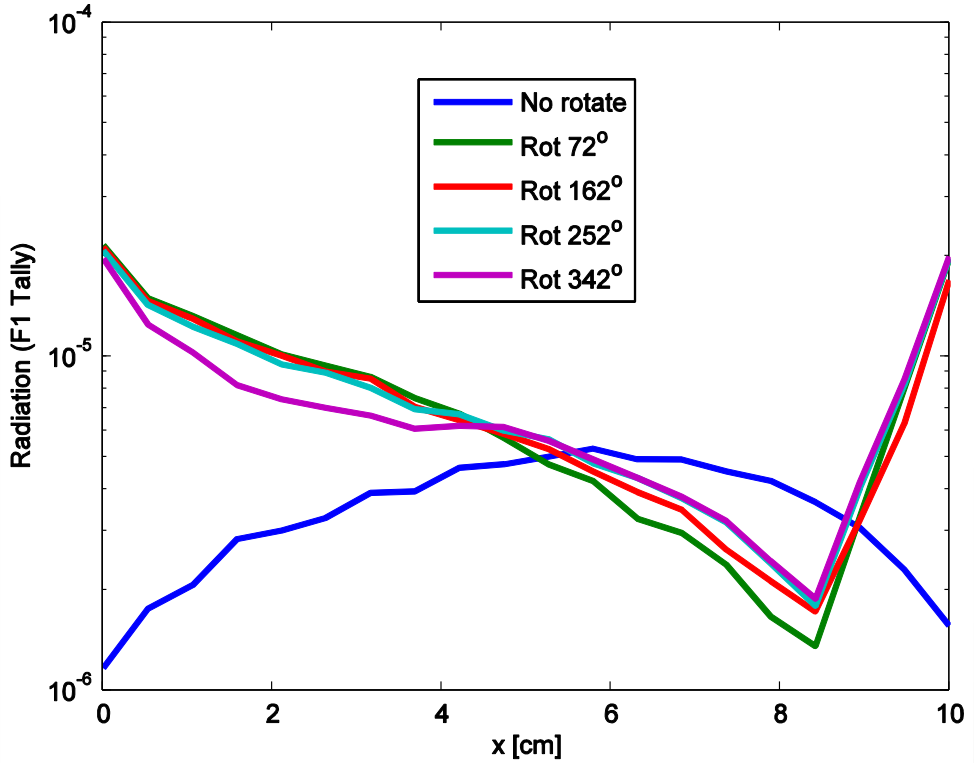
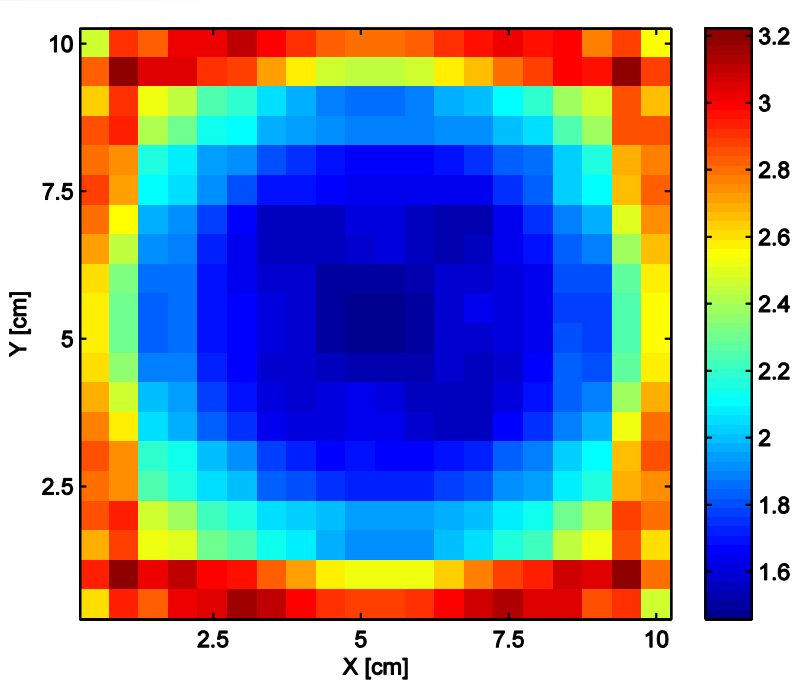
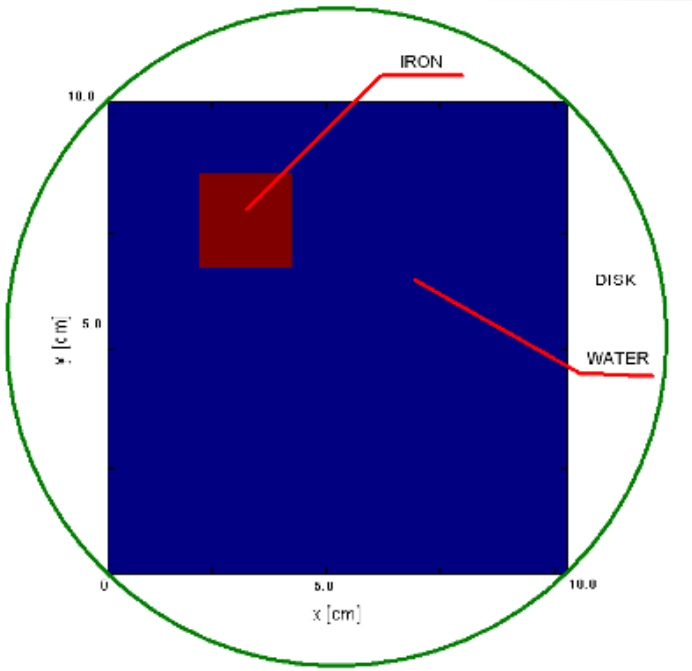


Fig: Transmitted radiation measured with object rotated in different angle.

Failure of Analytic Method to Reconstruct Total Cross Section Image for Model Problem

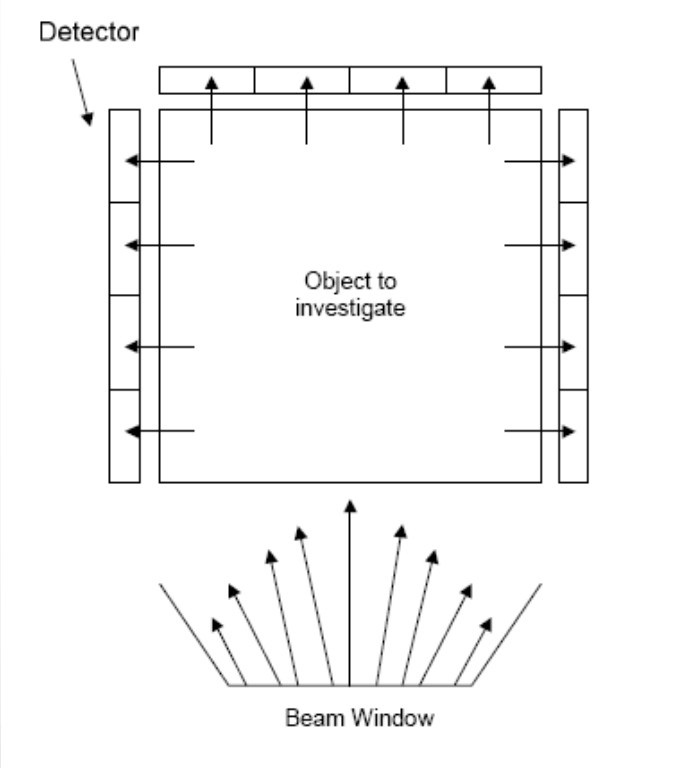


Total cross section reconstructed with FBP method for the test problem.



Geometry and material configuration of the model problem.

Gradient-based Deterministic Optimization Method



A schematic diagram of the beam-object-detector system

- Objective function

$$\Phi = \frac{1}{2}\sum_{i=1}^{N}\left(P_i - M_i\right)^2$$

- Here '*M*' is experimental measurements provided by MCNP model
- '*P*' is predicted measurements provided by forward model calculation, which is treated as a function of properties of the unknown object

$$P = P\left(\sigma_t, \sigma_s, \sigma_{s1}, \cdots\right)$$

$$\Rightarrow \Phi = \Phi\left(\sigma_t, \sigma_s, \sigma_{s1}, \cdots\right)$$

Forward and Inverse Model

- Forward model: One-group neutron transport equation for a non-multiplying system with linearly anisotropic scattering

$$\underline{\Omega}\bullet\underline{\nabla}\psi(\underline{r},\underline{\Omega},t)+\Sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega},t)=\frac{1}{4\pi}\Sigma_s(\underline{r})\left[\phi(\underline{r},t)+3g\underline{\Omega}\bullet\underline{J}(\underline{r},t)\right]+S_{ext}(\underline{r},\underline{\Omega},t)$$

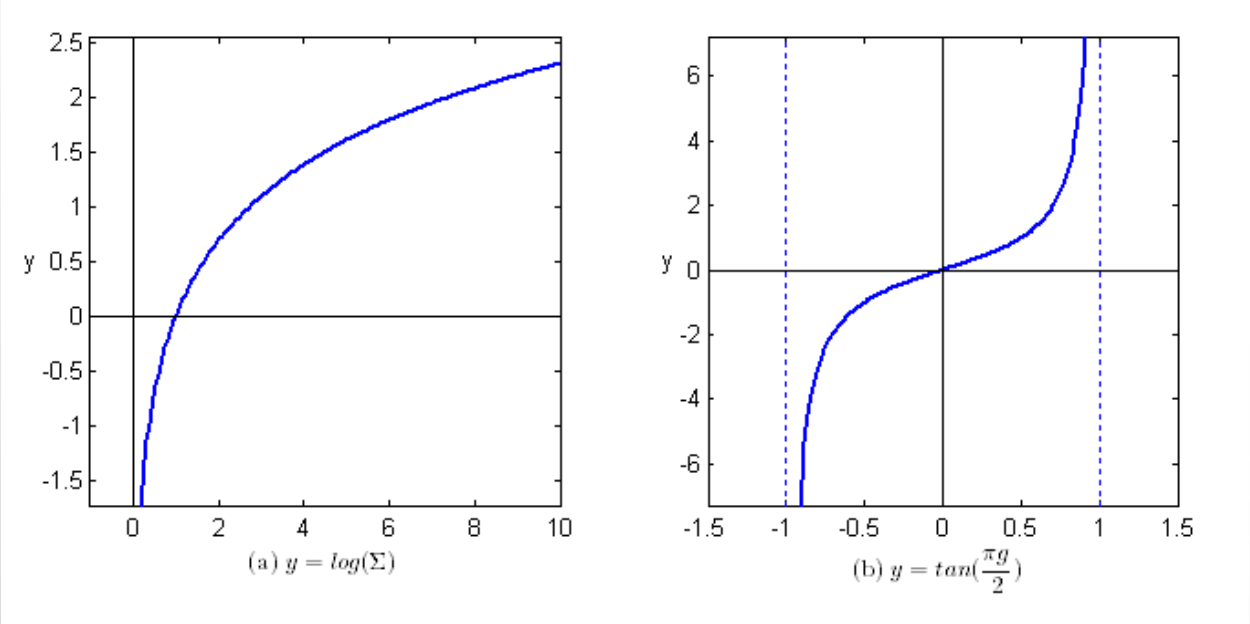
- Inverse model: Nonlinear conjugated gradient (CG) based iterative updating scheme

1. *Initialize variables* $\mathbf{x}^{(1)}$, *search direction* $\mathbf{d}^{(1)}=\mathbf{r}^{(1)}$, *where* $\mathbf{r}^{(1)}\equiv-\nabla\Phi\left(\mathbf{x}^{(1)}\right)$, $\mathbf{x}=\{\Sigma_t,\Sigma_s,g\}$
2. *Define termination tolerance* ε *and set iteration counter* $k=0$
3. *Start of iteration loop*
4. *Perform line search to find* $\alpha_{\min}$ *that minimizes* $\Phi(\mathbf{x}^{(k)}+\alpha\mathbf{d}^{(k)})$
5. $\mathbf{x}^{(k+1)}=\mathbf{x}^{(k)}+\alpha_{\min}\mathbf{d}^{(k)}$
6.
7. $\mathbf{r}^{(k+1)}\equiv-\nabla\Phi\left(\mathbf{x}^{(k+1)}\right)$
8. $\mathbf{d}^{(k+1)}=\mathbf{r}^{(k+1)}+\beta_k\mathbf{d}^{(k)}$
9.
10. $k=k+1$
11. *Exit if* $\left\|\nabla\Phi\left(\mathbf{x}^{(k)}\right)\right\|<\varepsilon$
12. *End of iteration loop*

Variable Change Technique

Purpose: Convert constrained optimization to non-constrained optimization

$$x_i^{(k+1)} = x_i^{(k)} + \alpha_{x,step} d_i^{(k)}, \quad (x = \Sigma \text{ or } g)$$



(a) $y_j = \log(\Sigma_j) \Rightarrow$

$$\frac{\partial \Phi}{\partial y_j} = \frac{\partial \Phi}{\partial \Sigma_j}\frac{d\Sigma_j}{dy_j} = \frac{\partial \Phi}{\partial \Sigma_j}\Sigma_j$$

(b) $y_j = \tan\left(\frac{\pi}{2} g_j\right) \Rightarrow$

$$\frac{\partial \Phi}{\partial y_j} = \frac{\partial \Phi}{\partial g_j}\frac{dg_j}{dy_j}$$

$$= \frac{\partial \Phi}{\partial g_j}\frac{2}{\pi}\frac{1}{1+\tan^2\left(\frac{\pi}{2} g_j\right)}$$

$$y_i^{(k+1)} = y_i^{(k)} + \alpha_{y,step} d_{y,j}^{(k)}$$

Nonlinear CG Updating Scheme with Variable Change Technique Incorporated

1. *Initialize variables* $\mathbf{x}^{(1)}$*, search direction* $\mathbf{d}^{(1)} = \mathbf{r}^{(1)}$ *, where* $\mathbf{r}^{(1)} \equiv -\nabla\Phi\left(\mathbf{x}^{(1)}\right),\ \mathbf{x} = \{\Sigma_t, \Sigma_s, g\}$
2. *Define termination tolerance* ε *and set iteration counter* $k = 0$
3. *Start of iteration loop*
4. *Change variable x to y*
5. *Perform line search to find* $\alpha_{\min}$ *that minimizes* $\Phi(\mathbf{y}^{(k)} + \alpha\mathbf{d}^{(k)})$
6. $\mathbf{y}^{(k+1)} = \mathbf{y}^{(k)} + \alpha_{\min}\mathbf{d}^{(k)}$
7. $\mathbf{r}^{(k+1)} \equiv -\nabla\Phi\left(\mathbf{y}^{(k+1)}\right)$, where $\nabla\Phi\left(\mathbf{y}^{(k+1)}\right)$ is calculated based on $\nabla\Phi\left(\mathbf{x}^{(k+1)}\right)$
8.
9. $\mathbf{d}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta_k\mathbf{d}^{(k)}$
10. $k = k + 1$
11. *Change variable y back to x*
12. *Exit if* $\left\|\nabla\Phi\left(\mathbf{x}^{(k)}\right)\right\| < \varepsilon$
13. *End of iteration loop*

Deterministic Optimization Results for the Model Problem

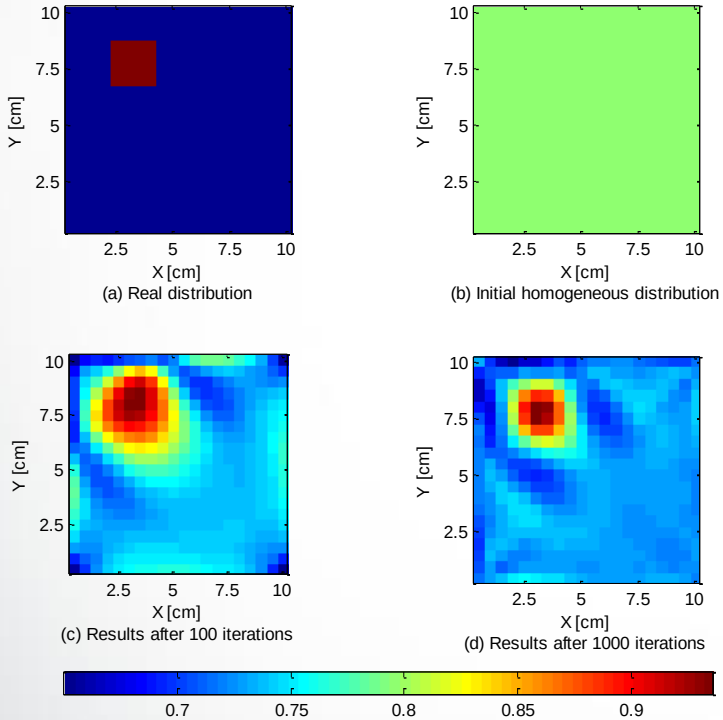
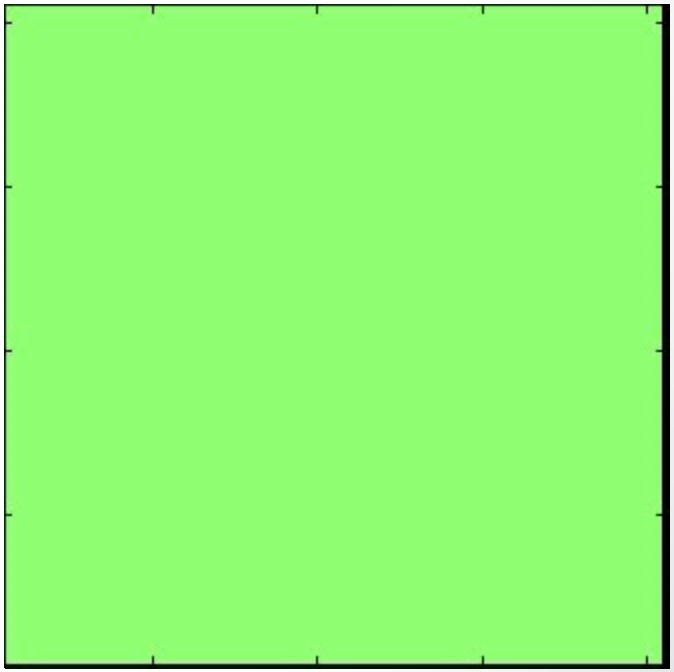


Fig: Transport cross section (Σ_{tr}) distribution obtained from deterministic CG based iterative search scheme for the one iron problem. (a) The real Σ_{tr} (background is water and square inclusion is iron). (b) Initial guess for Σ_{tr} . (c) and (d) are results after 100 and 1000 iterations, respectively.



Animation show of the transport cross section (Σ_{tr}) distribution within the object changes after each updating iteration.

Model Problem II

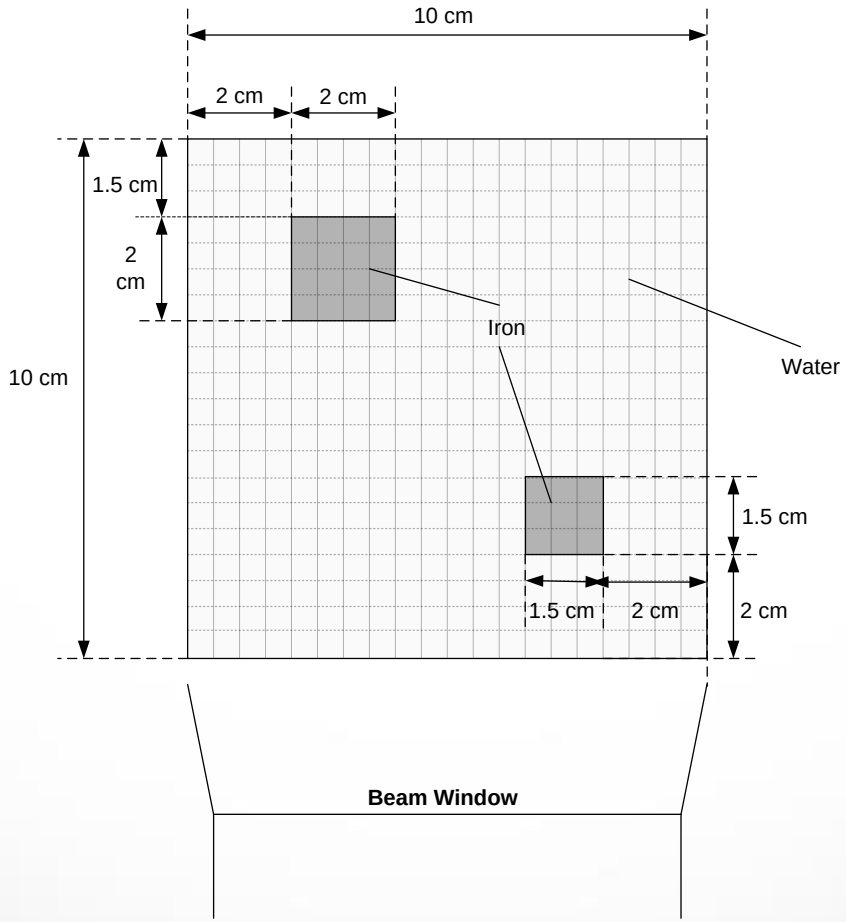


Fig: Schematic diagram of the two irons inclusion model problem (X-Y view).

Optimization Results for Model Problem II

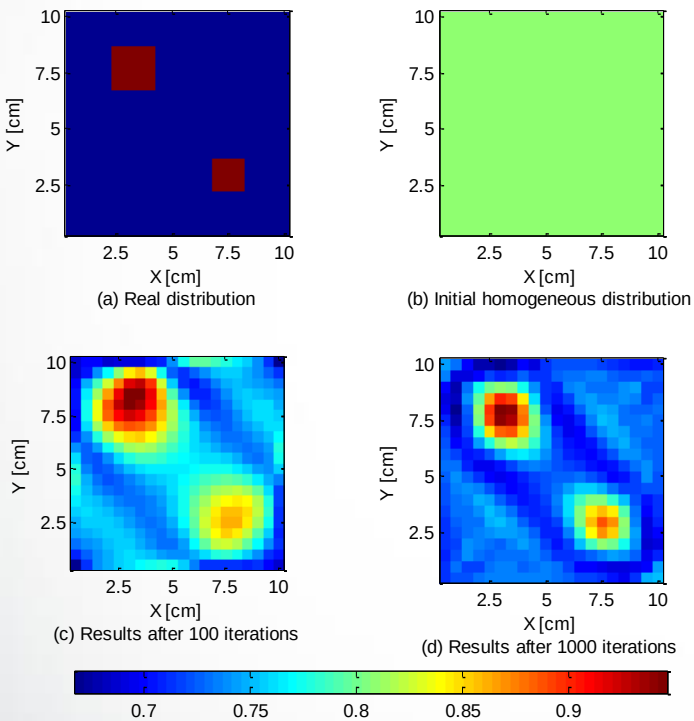
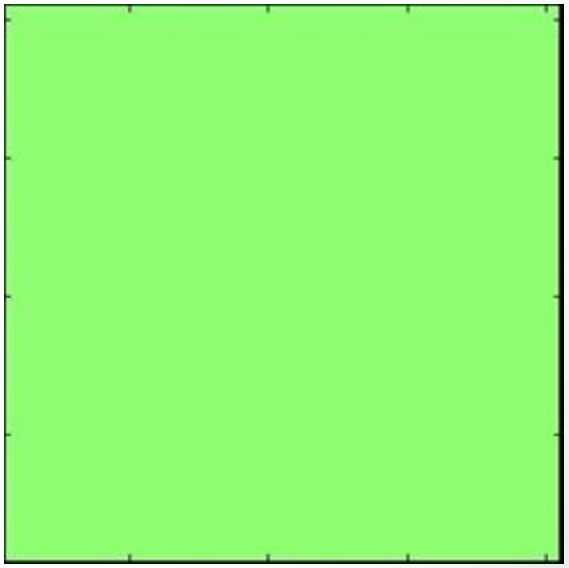


Fig.: Transport cross section (Σ_{tr}) distribution obtained from deterministic CG based iterative search scheme for the two irons problem. (a) The real Σ_{tr} (background is water and square inclusions are irons). (b) Initial guess for Σ_{tr} . (c) and (d) are results after 100 and 1000 iterations, respectively.



Animation show of the reconstruction procedure for transport cross section (Σ_{tr}) distribution within the object changes with each iteration.

Conclusions for Inverse Problem

- Some advances in inverse transport method are developed and successfully applied to solve 2D neutron tomography problem
- Optically think problems with a high scattering ratio, in which analytic tomography method generally fails, are effectively solved with gradient based iterative optimization method
- An easy implemented variable change technique is introduced to convert constrained optimization into unconstrained on in inverse transport applications
- Results from our simple neutron tomography problems demonstrate that the method works well and is robust.
- Future investigation for this research is to address measurement noise and model error, provide adaptive mesh refinement capability to forward model, extend to multi-group transport model, etc.

Summary of this Talk

- Neutronics analysis in nuclear engineering is briefly introduced, the outstanding challenges and standard methods to tackle them are addressed
- Three research topics focus on different applications in nuclear engineering are presented, and they all can be casted as modeling and simulation (M&S) techniques in neutronics analysis area
- Difficulties problems in current work are discussed, and some potential research interest for future investigations is suggested as well

Selected Publications

1. Zeyun Wu, C. B. Kennedy, and H. S. Abdel-Khalik, “GPT-free Sensitivity Analysis for Monte Carlo Models,” *Nuclear Technology*, Submitted, July (2012)
2. Zeyun Wu and Hany S. Abdel-Khalik, “Further GPT-free Developments for Monte Carlo Models,” *Transactions of the American Nuclear Society*, **107** (2012).
3. Zeyun Wu, C. B. Kennedy, and H. S. Abdel-Khalik, “Application of GPT-Free Method to Sensitivity Analysis in Monte Carlo Models,” *Transactions of the American Nuclear Society*, **106** ,763-766 (2012).
4. Zeyun Wu, Qiong Zhang and Hany S. Abdel-Khalik, “On Hybrid Monte Carlo-Deterministic Methods for Reactor Analysis,” *Nuclear Technology*, **180**(3) (2012).
5. Zeyun Wu and Hany S. Abdel-Khalik, “Hybrid Biasing Approaches for Global Variance Reduction,” *Applied Radiation and Isotopes*, Accepted for publication, (2011).
6. Zeyun Wu, Qiong Zhang and Hany S. Abdel-Khalik, “A Hybrid Variance Reduction Method Based on Gaussian Process for Core Simulation,” *Transactions of the American Nuclear Society*, **105**, 872-874 (2011).
7. Zeyun Wu and Marvin L. Adams, “Advances in Inverse Transport Methods,” *Proceedings of 18th International Conference on Nuclear Engineering*, 2, Paper no. ICONE18-29835, 713-719 (2010).
8. Zeyun Wu and Marvin L. Adams, “Variable Change Technique Applied to Constrained Inverse Transport Applications,” *Transactions of the American Nuclear Society*, **102**, 209-212 (2010).