A Hybrid Variance Reduction Method Based on Gaussian Process for Nuclear Reactor Analysis

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Introduction

- 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)

Challenges

- 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

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

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

Motivations of GP Approach

- **<u>Importance</u>** for different responses are expected to be correlated albeit they are different.
- Resulting responses **<u>uncertainties</u>** are expected to be correlated
  - Given *m* responses, let *r* denote number of independent correlations.
  - Bias MC particles towards *r (rather than m)* independent correlations
- Gaussian Process (GP) approach is developed on these ideas

Correlations?

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

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

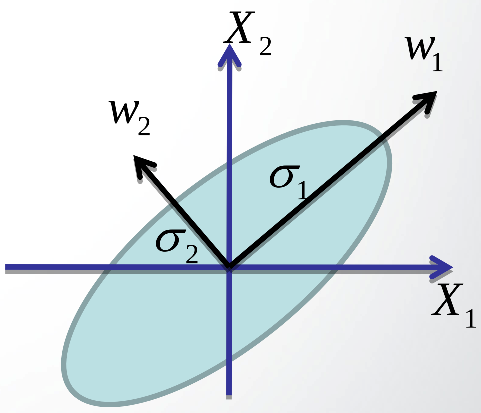
$$\mathbf{C} = \mathbf{W}\boldsymbol{\Sigma}^2\mathbf{W}^T \approx \mathbf{W}_r\boldsymbol{\Sigma}_r^2\mathbf{W}_r^T$$

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

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

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

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



Gaussian Process (GP) Approach

- Radiation transport may be treated as a Gaussian Process[1]
- If responses correlations (covariance matrix) can be constructed and effective rank *r* can be estimated, one can reduce it to identify *r* uncorrelated pseudo responses
- *r* pseudo responses are formed in **GP** approach

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

[1]M. KENNEDY and A. O'HAGAN, "Bayesian calibration of computer model," *Journal of the Royal Statistical Society*, **63**, 3, 425–464 (2001).

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:

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

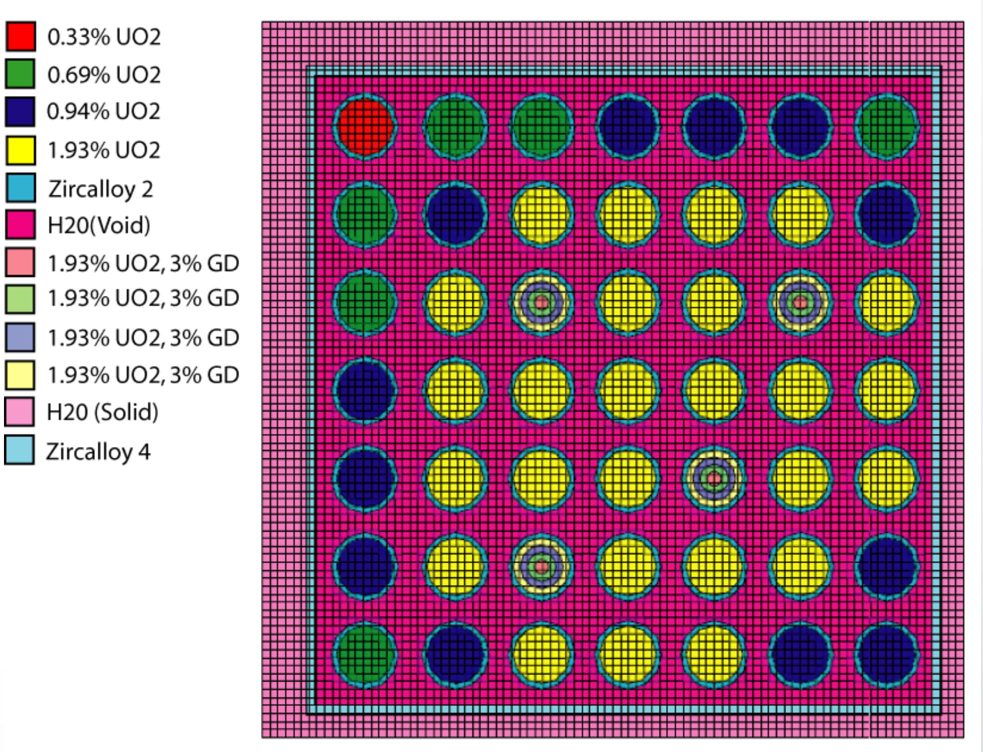
The covariance information between all pairs of *m* responses may also be represented by a symmetric covariance matrix $\mathbf{C} \in \mathbf{R}^{m \times m}$ such that: $\mathbf{C}_{ij} = \operatorname{cov}(R_i, R_j)$. The SVD form of this matrix is:

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

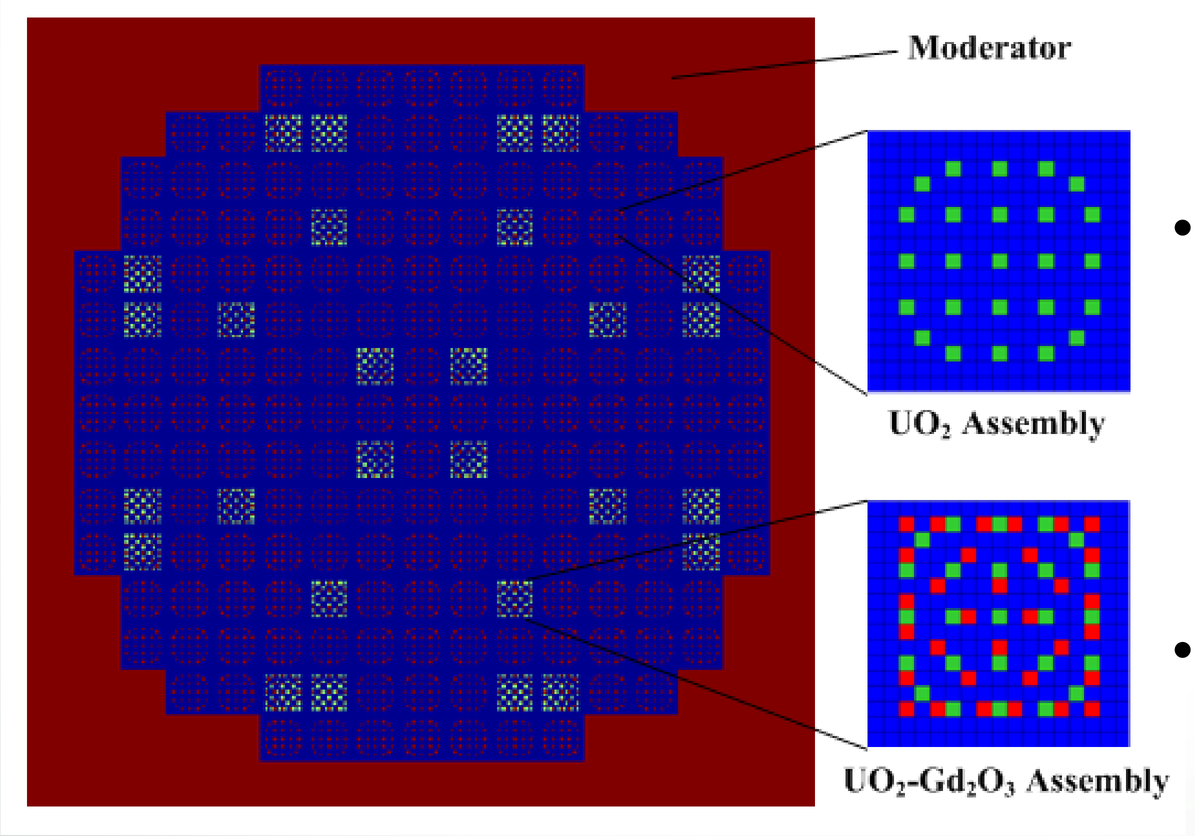
Numerical Applications

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

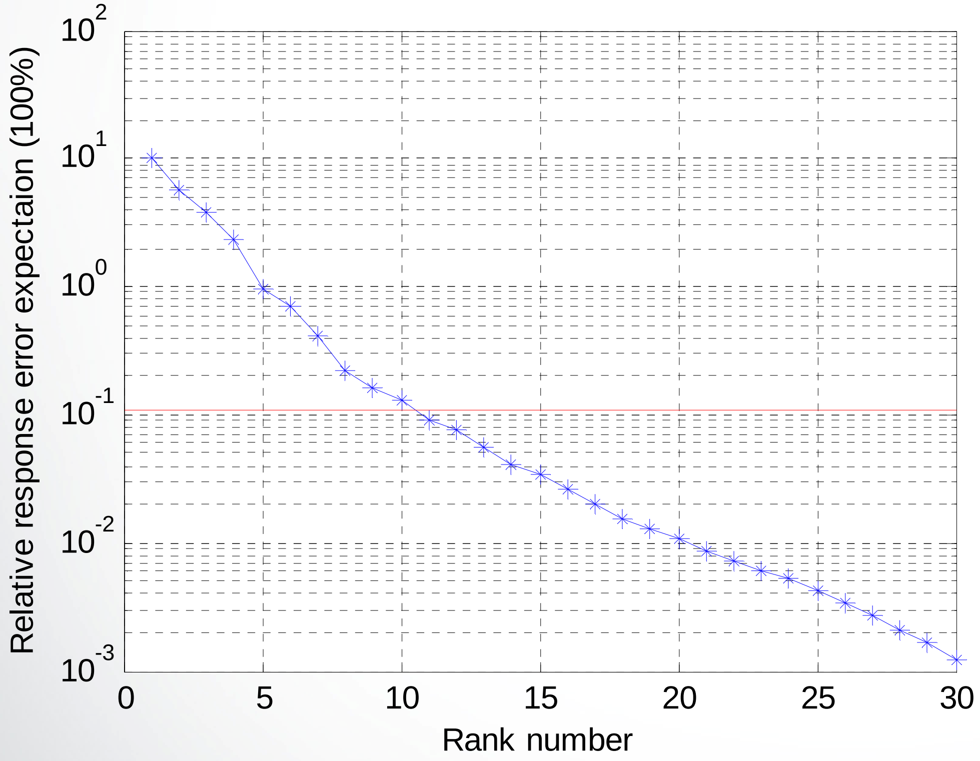


Case Study 2: PWR Core Model



- 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.

Estimate of the Effective Rank for Covariance Matrix



SVD of Covariance Matrix:

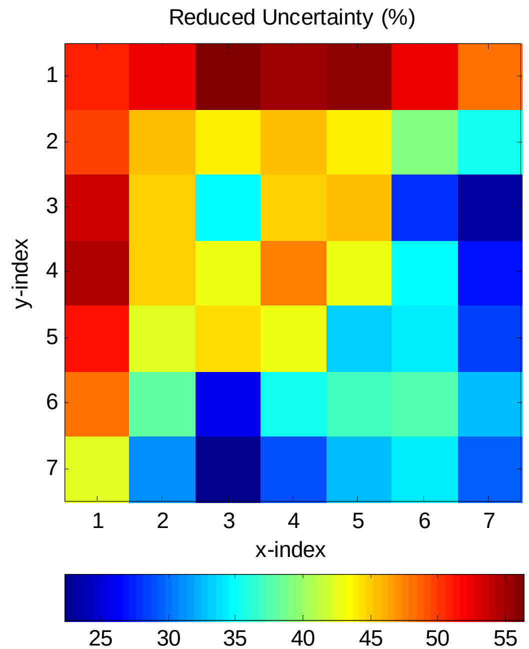
$$\mathbf{C} = \mathbf{W}\mathbf{\Sigma}^2\mathbf{W}^T = \sum_{i=1}^{m} \sigma_i^2 \vec{w}_i \vec{w}_i^T$$

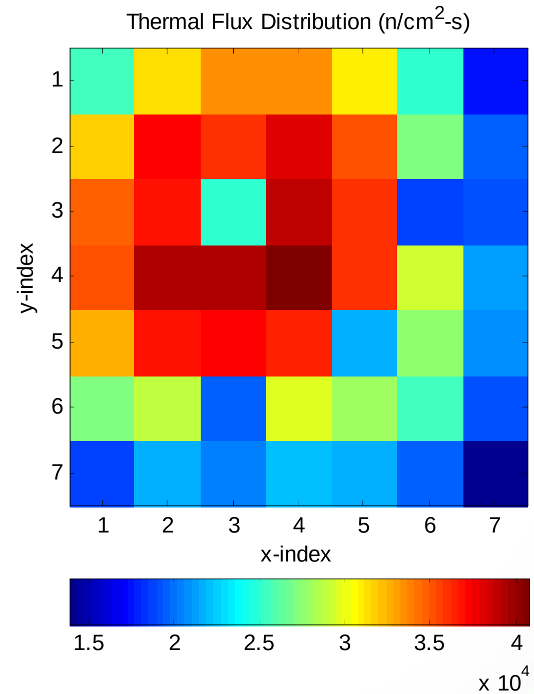
Truncated SVD Approximation:

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

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

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



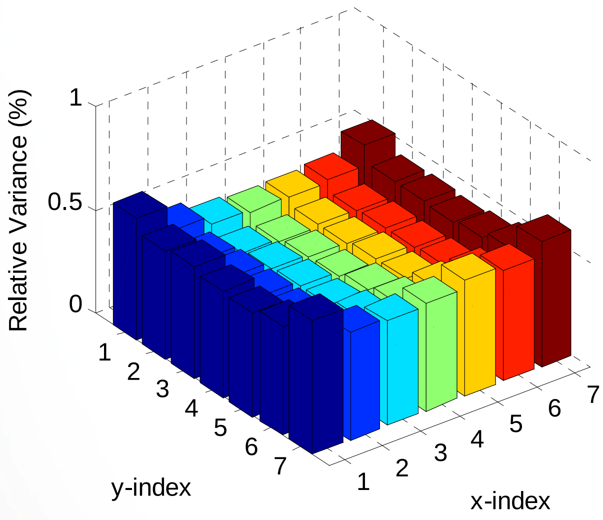


a. Standard Deviation Reduction

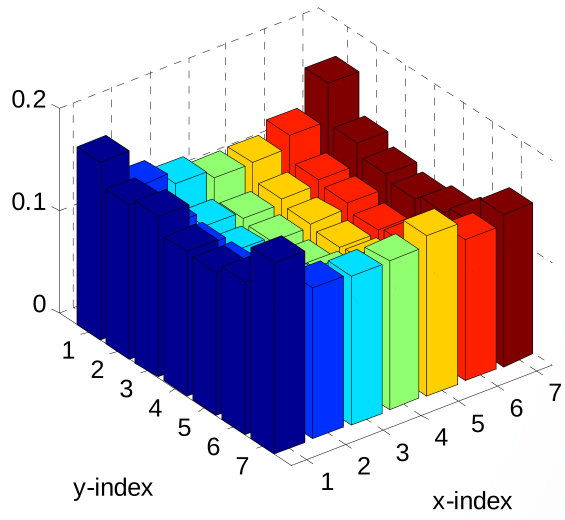
b. Mean Thermal Flux Distribution

Metric: $\varepsilon_i = \dfrac{\sigma_i^{\text{FW-CADIS}} - \sigma_i^{\text{GP}}}{\sigma_i^{\text{FW-CADIS}}} \times 100\%$

Global Uniformity of Variance (GP vs. FW-CADIS, Assembly Model)

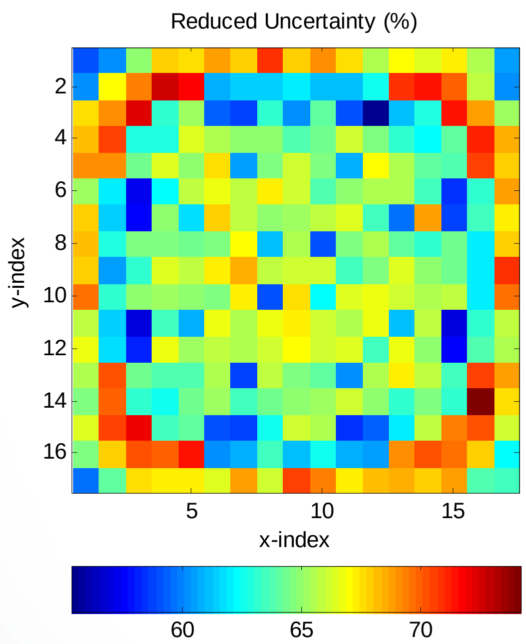


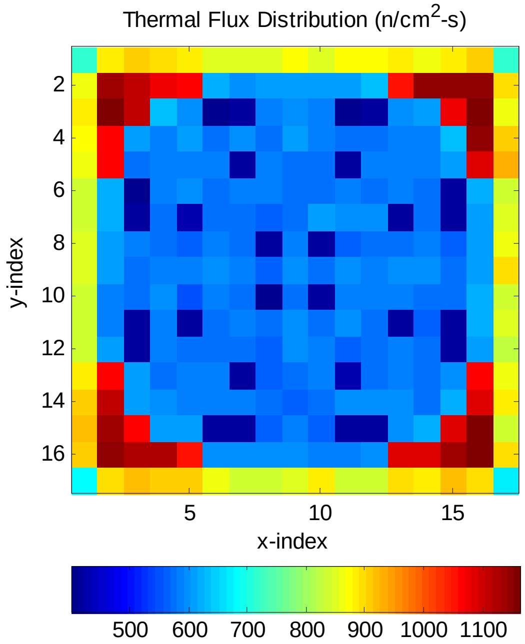
a. FW-CADIS Approach



b. GP Approach

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





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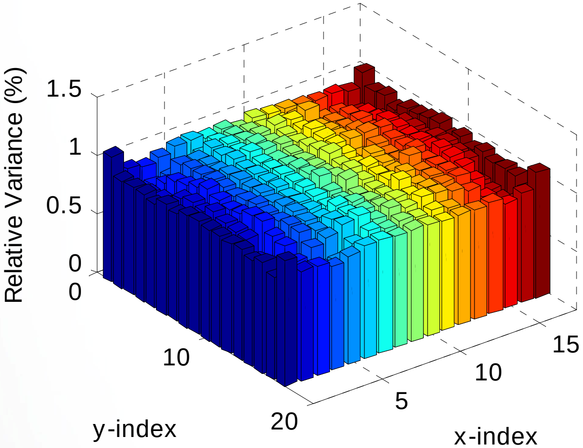

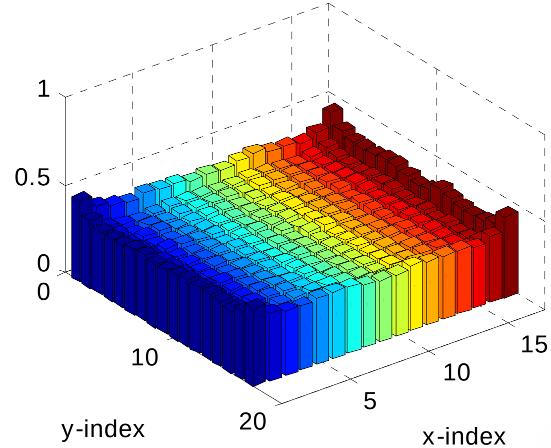

a. FW-CADIS Approach

b. GP Approach

Conclusions

- Number of independent correlations are much smaller than number of responses, when responses are required everywhere in phase space
- GP assumption provides one way to take advantage of responses uncertainties correlations and the deterministic models can be employed to identify correlations
- Simple numerical experiments show that GP approach successfully gain better convergence in MC simulation comparing to FW-CADIS approach
- This idea could be extended to other hybrid deterministic-MC techniques
- A hybrid between GP and FW-CADIS methodology is suggested to reach their combined benefits in the future