A Hybrid Variance Reduction Method Based on Gaussian Process for Core Simulation

Zeyun Wu, Qiong Zhang and Hany S. Abdel-Khalik

Department of Nuclear Engineering, North Carolina State University, Raleigh, NC 27695
{zwu3, qzhang7, abdelkhalik}@ncsu.edu

INTRODUCTION

Variance reduction techniques is usually employed to accelerate the convergence of Monte Carlo (MC) simulation. Hybrid deterministic-MC methods [1, 2, 3] have been recently developed to achieve the goal of global variance reduction. Hybrid methods employ deterministic models (both forward and adjoint) to bias source particles and assign appropriate importance map to MC models. If done properly, hybrid methods have been shown to accelerate the convergence of MC simulation - that is obtaining acceptable reduction in the statistical uncertainties for the responses of interest with less computational overhead.

Under the assumption that the statistical uncertainties resulting from the radiation transport may be treated as a Gaussian Process (GP) [4], a new hybrid approach for global variance reduction was presented in an earlier publication [5]. The principle behind this approach is recalled here along with a comparison to FW-CADIS method [6, 7], which is currently implemented in the SCALE package [8]. Unlike previous work, in which the covariance matrix describing the Gaussian process was calculated using analog MC calculation, this summary estimates the covariance matrix using a deterministic model. In previous work, MC model was used as a proof of principle, but in realistic calculations, the covariance matrix must be estimated inexpensively, hence the need to approximate it using a deterministic model. The construction of the covariance matrix as needed by the GP method is implemented in the MAVRIC sequence of SCALE to facilitate the comparison of the GP and the FW-CADIS approaches. Building on the work presented before which focused on simplified BWR assembly models [5], we apply the GP approach to a higher dimensional problem representing a prototypical PWR core model.

MATHEMATICAL DESCRIPTION

GP theory assumes that random fluctuation of a response follows a process that can be described by a normal distribution. If the statistical uncertainties for all responses of interest (say the group fluxes everywhere in the domain) can be treated as GPs, one could describe the correlations between these uncertainties via a covariance matrix. If this matrix is diagonal and well-conditioned, it implies that all responses have independent uncertainties, and hence no single biasing technique can be used to reduce all of them simultaneously. However, if the matrix is dense and ill-conditioned, one could in principle reduce the computational overhead required to reduce the uncertainties everywhere by taking advantage of their correlations. The lower the effective rank of the covariance matrix, the more correlations between responses, and the less computational overhead needed to reduce the variances globally.

Details on the GP methodology may be found in authors' previous summary [5]. The main contribution of this summary is to construct the covariance matrix $\mathbf{C}$ by employing inexpensive deterministic model. To simulate statistical uncertainty using a deterministic model, recall that the interaction between a neutron and a target nucleus is a random process whose probability is characterized by cross-sections. By sampling cross-sections randomly, one can estimate how the responses are correlated and hence construct an approximate covariance matrix.

The covariance matrix $\mathbf{C}$ is constructed by performing l deterministic forward model executions. Denote the n responses, generated in the jth model execution, by a vector $\vec{r}_j$, where $j = 1, 2, ..., l$. After l executions, the estimator for covariance matrix may be constructed as follows:

$$\mathbf{C} = \frac{1}{l-1}\sum_{i=1}^{l}\left(\vec{r}_j - \hat{\vec{r}}\right)\left(\vec{r}_j - \hat{\vec{r}}\right)^T, \tag{1}$$

where $\hat{\vec{r}}$ is a vector of estimated means of all responses, e.g.

$$\hat{\vec{r}} = \frac{1}{l}\sum_{j=1}^{l}\vec{r}_j\ .$$

The covariance matrix $\mathbf{C}$ may also be rewritten via singular value decomposition (SVD) as follows [9]:

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

where $\mathbf{W} = \left[\vec{w}_1 \quad \vec{w}_2 \quad .... \quad \vec{w}_n\right] \in \mathbf{R}^{n\times n}$ is a matrix of n orthonormal singular vectors, $\mathbf{\Sigma} = \text{diag}\{\sigma_1, \sigma_2, ..., \sigma_n\}$ is a diagonal matrix of n nonzero singular values. The covariance matrix $\mathbf{C}$ can also be approximated with truncated SVD approach as follows:

$$\mathbf{C}_r = \mathbf{W}\mathbf{\Sigma}\mathbf{W}^T = \sum_{i=1}^{r}\sigma_i\vec{w}_i\vec{w}_i^T, \tag{3}$$

where r is known as the effective rank of the covariance matrix. The effective rank is estimated utilizing the inequality as follows:

$$\|\mathbf{C} - \mathbf{C}_r\| < \delta\ , \tag{4}$$

where δ is a user-defined tolerance. After the decomposition in Eqn. (2) is calculated and the effective rank r is determined by Eqn. (4), the GP approach formulates r pseudo responses of the form:

$$\xi_j^{\mathrm{GP}} = \vec{w}_j^{\,T}\vec{r},\ j = 1, 2, ..., r\ . \tag{5}$$

Here r is the effective rank of the unknown covariance matrix and $\vec{r}$ represents the response vector. The MAVRIC sequence is then executed to bias the MC solution to minimize the variance of the pseudo responses. The premise is that by reducing the variance of the pseudo responses, the variances of all original responses are simultaneously reduced because of the correlations.

Note that in the FW-CADIS approach, only one adjoint and one forward model executions are required. The GP approach however requires at least r forward flux executions to construct the covariance matrix. Moreover, it requires r different adjoint calculations to bias the solution towards the various pseudo responses. These additional adjoint runs have to be considered when comparing figure of merits.

It is important to address that the potential value of the GP approach can be realized for models with high dimensional phase space and many responses. Like any projection approach, the potential for reduction increases as the dimensionality of the model increases. When only few responses are required however, it is better to design weight window maps that target the responses of interest only. Our primary interest focuses on two applications: using MC models to generate the few-group cross-sections for core wide calculations. In this case, thousands of assembly calculations must be completed. Given the correlations between these models, a huge reduction in the computational overhead may be possible. The other application is core-wide MC models where the flux is required everywhere in the phase space.

REACTOR CORE STUDY

A prototypical PWR full core model is developed with the standard SCALE geometry utility. It is designed as a slight variation to the benchmark problems presented in [10] and [11]. The full core model consists of 193 fuel assemblies (blue regions in Fig. 1) laid out in a 17×17 grid scheme and surrounded by light water (red regions in Fig. 1). The cubic volume of the whole active core is 365.6×365.6×335.3 cm^3. The cubic volume of each assembly is 21.505×21.505×335.28 cm^3. Two types of fuel assemblies are modeled (blue regions): a UO_2 fuel assembly and a UO_2-Gd_2O_3 fuel assembly. The loading pattern of the full core is shown in the Fig. 1. Each assembly consists of a 17×17 grid of pin cells with each pin cell measuring 1.265×1.265 cm in the X-Y plane.

The singular values of the covariance matrix are shown in Fig. 2. A cutoff of r=12 (red horizontal line) is selected such that the error in Eqn. (4) does not exceed the desired statistical uncertainties for the responses.

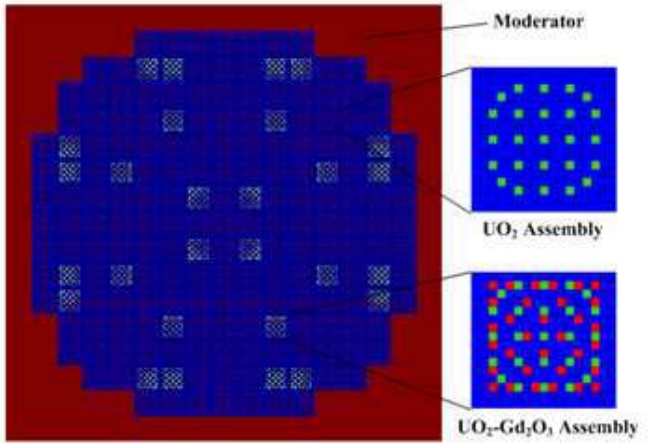

Fig. 1. X-Y View of the active core model with details assembly described on the side.

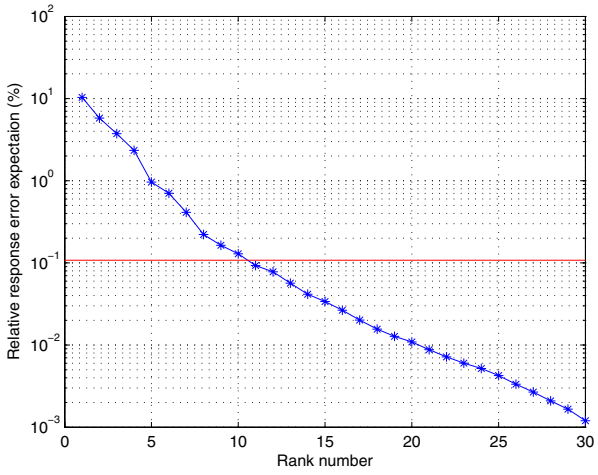

Fig. 2. Covariance Matrix Singular Values.

To compare the FW-CADIS and GP approach, a simple metric is employed which described the relative reduction in standard deviation defined as follows:

$$\varepsilon = \frac{\sigma^{\text{FW-CADIS}} - \sigma^{\text{GP}}}{\sigma^{\text{FW-CADIS}}} \times 100 \tag{6}$$

No figure of merit comparisons were done in this study, as MC calculations dominated the total computational time (MC computer time in the order of hours, versus deterministic time in the order of seconds). In the future, a more complete comparison based on figure of merit type metric to help compare the various approaches. This follows as future work will focus on eigenvalue problem, where deterministic models are expected to take more time especially for high dimensional problems.

Results in Fig. 3 show that the standard deviations in GP method are reduced on the average by a factor two as compared to the FW-CADIS method. This indicates the potential of GP approach to reduce the variance globally by

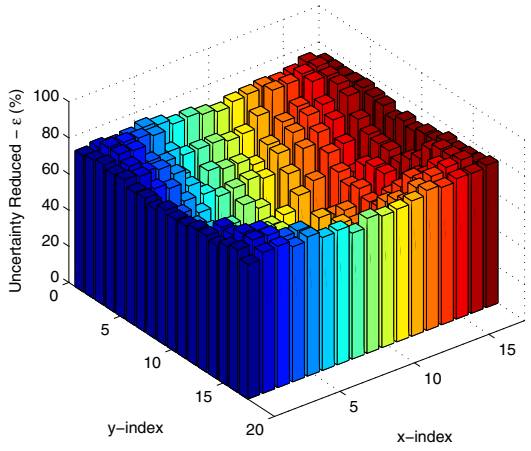

Fig. 3. FW-CADIS vs. GP.

taking advantage of the correlations between the statistical uncertainties of the responses.

Note that the process we employed here is the simplest approach to taking advantage of responses correlation. In effect, the GP approach has reduced the number of original responses to r pseudo responses which have been reduced separately using adjoint-based weight windows. Other clever approaches could be attempted. For example, a FW-CADIS type approach could be employed to combine the pseudo-responses by scaling each pseudo response by an appropriately selected pseudo flux. Another approach is to employ a subspace approach to randomly combine the pseudo responses [12]. One more approach may combine the pseudo responses by scaling each one based on its associated singular values. All these approaches have the potential of optimizing the behavior of this approach.

CONCLUSIONS

A new approach based on Gaussian Process theory for global variance reduction is presented and the results compared to the FW-CADIS method. GP method takes advantage of the correlations between the variances of the various responses which are described by a covariance matrix. Deterministic calculations are employed to construct an estimate of the covariance matrix by randomly sampling cross-sections.

A full core model is implemented and analyzed in the current study. A significant rank reduction is observed for the covariance matrix, implying that only few adjoint evaluations are needed to perform global variance reduction.

Current work has focused on fixed-source problem only. The ultimate goal of our work is the application of global variance reduction to eigenvalue problems which represents the focus of ongoing efforts.

Finally, future work will focus on optimizing the GP approach by hybridizing it with FW-CADIS and/or subspace approach.

ACKNOWLEDGMENTS

This work has been funded by the Department of Energy (DOE) via a Nuclear Energy University Program (NEUP) grant.

REFERENCES

1. A. HAGHIGHAT and J. WAGNER, "Monte Carlo Variance Reduction with Deterministic Importance Functions," *Progress in Nuclear Energy*, **42**, 1, 25–53 (2003).
2. J. DENSMORE and E. LARSEN, "Variational variance reduction for particle transport eigenvalue calculations using Monte Carlo adjoint simulation," *Journal of Computational Physics*, **192**, 2, 387–405 (2003).
3. T. BECKER, A. WOLLABER, and E. LARSEN, "A Hybrid Monte Carlo-Deterministic Method for Global Particle Transport Calculations," *Nuclear Science and Engineering*, **155**, 2, 155–167 (2007).
4. M. KENNEDY and A. O'HAGAN, "Bayesian calibration of computer model," *Journal of the Royal Statistical Society*, **63**, 3, 425–464 (2001).
5. Q. ZHANG and H. S. ABDEL-KHALIK, "Gaussian Process Approach for Global Variance Reduction," *Trans. Am. Nucl. Soc. Meeting, Hollywood, FL* (June 2011).
6. J. WAGNER, E. BLAKEMAN, and D. PEPLOW, "A Forward-Weighted CADIS Method for Global Variance Reduction," *Trans. Am. Nucl. Soc. Meeting, Washington, D.C.*, **97** (Nov. 2007).
7. J. WAGNER, E. BLAKEMAN, and D. PEPLOW, "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions and Multiple Localized Quantities," *Proc. 2009 Int. Conf. Adv. Math. Comp. and Reactor Physics (M&C 2009), Saratoga Spring, NY* (2009).
8. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations, ORNL/TM-2005/39, Version 6, Vols. I-III, January 2009*.
9. G. GOLUB and V. L. C. F., *Matrix Computations (3rd ed.)*, John Hopkins (1996).
10. A. YAMAMOTO, I. T., I. T., and S. E., "Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels," *Journal of NUCLEAR SCIENCE and TECHNOLOGY*, **39**, 8, 900–912 (2002).
11. S. DOUGLASS, F. RAHNEMA, and J. MARGULIES, "A Stylized three dimensional PWR whole-core benchmark problem with Gadolinium," *Annals of Nuclear Energy*, **37**, 10, 1384–1403 (2010).
12. Q. ZHANG and H. S. ABDEL-KHALIK, "Hybrid Monte Carlo-Deterministic Approach for Global Variance Reduction," *Trans. Am. Nucl. Soc. Meeting, Hollywood, FL* (June 2011).