Further Development of Efficient Uncertainty Quantification Techniques for Core Simulation

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INTRODUCTION

Since the Nuclear Regulatory Commission (NRC)'s adoption of the best-estimate plus uncertainty methodology in the validation of computer codes, the need for rigorous, comprehensive, and efficient algorithms for quantification of uncertainty has greatly increased. With the complexity of reactor physics calculations, representing the focus of our study, the extant algorithms for uncertainty quantification (UQ) remain to be challenged due to the associated high computational and storage requirements. This summary presents our recent research on developing an efficient framework for propagation of nuclear data uncertainties in support of performing routine engineering core analysis. The goal is to establish an automated framework that takes uncertainties from the multi-group format and generate a compressed representation of few-group cross-section uncertainties that can be employed to perform core simulation calculations on a routine basis.

BACKGROUND

Focusing on propagation of cross-section uncertainties throughout the conventional sequence of Light Water Reactor (LWR) design calculations, our goal is to address the demanding computational burden spawned by the large size of the uncertainty space. The most straightforward UQ approach relies on stochastic sampling (Monte Carlo), adopted by Organization for Economic Cooperation and Development (OECD) Uncertainty Analysis in Modeling (UAM) benchmark framework for uncertainty analysis methodologies in reactor simulations [1]. In our context, this method generates random samples of the lattice physics input parameters (e.g., multi-group cross-sections) that are consistent with their prior uncertainties, as described by their prior covariance matrix. A straightforward implementation would generate reactor-specific few-group cross-section libraries along with their uncertainties covering the wide range of conditions employed in their functionalization. This turns out to be a herculean task when considering that the number of input parameters to a typical core simulator could range anywhere between tens of thousands to millions of parameters.

To address this challenge, practitioners are forced to make extreme simplifying assumptions about the few-group cross-sections, such as relaxing dependencies on historical and instantaneous core conditions, such as burnup, void and fuel temperature, and limiting the analysis to macroscopic core depletion models only; see for example Refs. [1], [2] and [3] for implementations incorporating some of these assumptions. The idea behind these approaches is to use representative cross-section uncertainties that approximate the true uncertainties over the range of conditions used for cross-section functionalization. By doing so, one can significantly reduce the total number of uncertainties to the order of ten parameters, representing, for example, the two-group macroscopic cross-sections for fission, absorption, diffusion coefficient, etc.

While these approaches have reduced the computational requirements to determine the few-group uncertainties, they share one challenge in common, that is the ability to judge the quality of the assumptions made to achieve the sought reduction. Said differently, there currently exists no mathematical approach to measure the errors resulting from the embedded simplifying assumptions at both normal and off-normal operating conditions. Thus, the overarching goal of this research is to develop a systematic approach to efficiently propagate nuclear data uncertainties in a manner that credibly quantifies the propagated uncertainties. Our approach employs reduced order modeling (ROM) to compress the size of the uncertainty space. The premise is that the discarded components of the uncertainty space have very small impact on the core attributes of interest, and this small impact can be upper-bounded mathematically with high probability via the use of range finding algorithms (RFA). Earlier work [4,6] has shown that LWR reactor physics models are inherently reducible which could be exploited to facilitate the propagation and prioritization of uncertainty sources.

Specifically, earlier work has investigated the effects of branch cases and depletion on the propagated uncertainties for single lattice. However, a typical LWR core consists of several different types of lattice designs, which necessitates large computational expense when employing a brute-force uncertainty analysis method. Thus, it is necessary to look into the correlations of uncertainties between lattices. The current work investigates the impact of cross-section dependence on the lattice type based on ROM techniques. Two different BWR lattices are employed in our analysis. Results indicate that the size of the compressed uncertainty space is not greatly impacted by the introduction of new lattices, implying the efficiency of the algorithm is not expected to degrade significantly with multiple lattices, which is typical in LWR cores.

METHODOLOGY AND MATHEMATICAL DISCRIPTIONS

In this work, the ROM technique is applied on the cross-section library to determine the reducibility of uncertainty space throughout the burnup steps and different lattice types, in which a linear transformation of the parameters is identified via a range finding algorithm (RFA) [5]. The RFA identifies a small subset of effective parameters in the transformed space that can be used to describe the majority of response variations.

The few-group cross-sections for core simulations are calculated through lattice physics transport solvers, with multi-group cross-sections as input, which can be described as:

$$y = f(x) \tag{1}$$

where $y \in \mathbf{R}^m$ represents the few-group cross-sections for core simulation, while $f(x)$ is the transport solver with the input multi-group cross-sections *x*. In conventional deterministic uncertainty analysis approaches, the covariance matrix of few-group cross-sections $\mathbf{C}_y$ can be represented in terms of sensitivity information $\mathbf{S} = dy/dx$, which describes the first order variations of the few-group cross-sections with respect to the multi-group cross-sections, and the covariance matrix of multi-group cross-sections $\mathbf{C}_x$, in what is commonly referred to as the "sandwich equation" [4]:

$$\mathbf{C}_y = \mathbf{S}\mathbf{C}_x\mathbf{S}^T \tag{2}$$

where $\mathbf{C}_y \in \mathbf{R}^{m\times m}$, *m* is the size of core simulation cross-section library.

With single lattice, *m* is the number of responses, i.e. few-group cross-section, generated by a single lattice calculation. When extending to multiple lattice types, *m* will multiply based on the number of lattices. The following compression approach can be generalized to multiple lattices in the same way.

Compressed Library based on RFA

Covariance matrix of the few-group cross-section library has the dimension of m^2, which represents the number of few-group cross-sections evaluated at all conditions required for core-wide calculations. To reduce the effective dimensionality of this uncertainty space, a ROM approach is proposed. ROM-based dimensionality reduction techniques provide a rigorous mathematical approach by which the uncertainty space can be effectively shrunk down to a manageable size to enable practical application of uncertainty analysis with the reduction errors upper-bounded with high confidence. The objective of ROM is to find a representation:

$$y_r = \mathbf{Q}_y y = f(\mathbf{Q}_x x) \tag{3}$$

so that the errors resulting from the reduction can be constrained by the preset tolerance ε:

$$\left\| f(x) - f(\mathbf{Q}_x x) \right\| \le \varepsilon \tag{4}$$

This representation implies two reductions, one at the multi-group level and another at the few-group level. In this work, we focus on the reduction in the few-group level only. The reduction in the few-group space is represented by the active DOFs, identified to be much smaller than the dimension of the uncertainty space, and can be used to approximate the covariance matrix. Thus, the idea is to store the covariance matrix in terms of the active DOFs rather than the original dimensions of the matrix. To identify these DOFs, we employ rank revealing decomposition of the form:

$$\mathbf{C}_y = \mathbf{U}\mathbf{\Sigma}_y\mathbf{U}^T \tag{5}$$

where the $\mathbf{U} \in \mathbf{R}^{m\times r}$ matrix has a number of columns equal to the active DOFs, denoted by *r*, and $\mathbf{\Sigma}_y \in \mathbf{R}^{r\times r}$ is a diagonal matrix, whose elements represent the variances of the active DOFs.

To determine the effective rank *r*, we use RFA algorithm [5], which is developed in earlier work to identify the best linear transformation with smallest number of active DOFs that can approximate the matrix $\mathbf{C}_y$ to a preset tolerance [6]. The detailed algorithm can be find in Ref. [4].

In reactor core calculation specification, we construct the sample space $\mathbf{Y}$ of few-group cross-sections, containing *N* random samples, each of which provided by one execution of lattice physics solver, as:

$$\mathbf{Y} = [y_1, y_2, \ldots, y_N],\ i = 1, 2, \ldots, N \tag{6}$$

where $y_i \in \mathbf{R}^m$ is made up of few-group homogenized cross-sections of all dependencies in one perturbation sample. The sample space may be rewritten using an orthogonal decomposition, such as singular value decomposition (SVD), expressed as:

$$\mathbf{Y} = \mathbf{U}\mathbf{S}\mathbf{V} \tag{7}$$

where $\mathbf{U} \in \mathbf{R}^{m\times s}$, $1 \le s \le N$, and the reconstructed reduced response spaces is described as:

$$\mathbf{Y}_r = \mathbf{U}_r\mathbf{S}_r\mathbf{V}_r,\ r = 1, 2, \ldots, s \tag{8}$$

The difference between $\mathbf{Y}$ and $\mathbf{Y}_r$ becomes smaller with larger rank *r*. With the preset tolerance ε, the effective rank can be determined with

$$\left\|\mathbf{Y}-\mathbf{Y}_r\right\| \le \varepsilon \qquad (9)$$

where $\|\bullet\|$ denotes for norms, so as the active subspace $\mathbf{U}_r \in \mathbf{R}^{m\times r}$.

NUMERICAL RESULTS

The numerical analysis in this summary focuses on the impact of multiple lattices on the homogenized few-group macroscopic cross-section uncertainties. The case study is based on two BWR lattice models with 7x7 fuel designs from Peach Bottom Unit 2 cycle 1, 2, 3 [7]. Fig. 1. and Fig. 2. depict the layout of Type 3c lattice model and Type 1 lattice model generated by NEWT [8]. Type 3c lattice consists of 2.50 wt % UO_2 fuel pins with Gd_2O_3 in 5 rods and Type 1 lattice is made up of 1.10 wt % UO_2 fuel pins without Gd_2O_3.

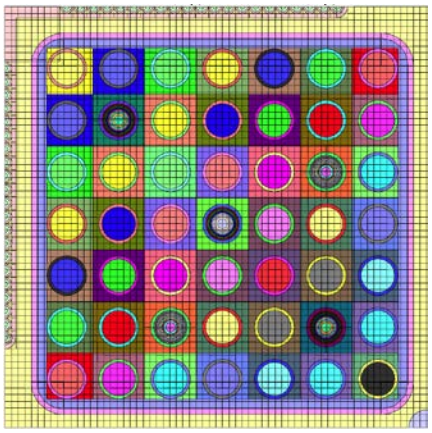

Fig. 1. Type 3c lattice model with NEWT.

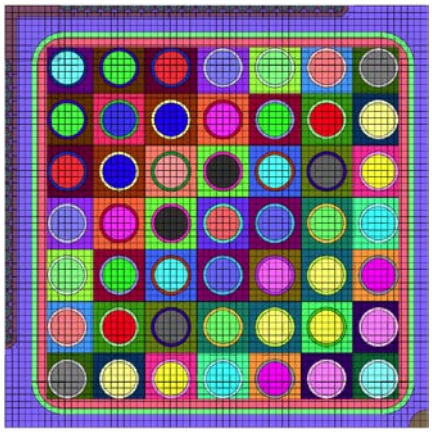

Fig. 2. Type 1 lattice model with NEWT.

The lattice physics is executed by TRITON [9] in SCALE 6.2b2 code package for fuel depletion, employing NEWT to solve neutron transport calculations. Multi-group cross-section libraries for both lattice models follow a 238-group energy structure. To investigate the reducibility of few-group cross-section uncertainty space among burnups and evaluate the impact of different lattice designs, both lattices are depleted to 70 GWD/MTU in 32 burnup steps and 96 random perturbed samples are generated for each lattice model by SAMPLER [10] sequence in SCALE to propagate cross-section uncertainties based on the SCALE 44-group covariance library. The responses selected for the uncertainty analysis are the assembly-wise homogenized 2-group macroscopic cross-sections. Five types of reaction, absorption, fission, transport, nu-fission and kappa-fission cross-sections are collected.

The uncertainty space of the homogenized few-group cross-sections generated by the lattice code will then be propagated to downstream core simulations to evaluate the uncertainties of core attributes. In this study, we employ NESTLE, which is a core simulator with few-group neutron diffusion equations spatially discretized utilizing the Nodal Expansion Method (NEM) [11], to model BWR full-core neutronics. NESTLE reads the 2-group homogenized macroscopic cross-sections output by TRITON in the form of polynomial coefficients as function of each branch cases. The macroscopic cross-section library for NESTLE in a given fuel color, burnup and control rod state can be described in terms of coolant density, coolant temperature, effective fuel temperature and soluble poison number density [11]:

$$\begin{aligned}\hat{\Sigma}_{xg} = a_{1_{xg}} &+ \sum_{n=1}^{2} a_{(n+1)_{xg}} (\Delta\rho_C)^n \\ &+ a_{4_{xg}} \Delta T_C + a_{5_{xg}} \Delta\sqrt{T_{F_{eff}}} + \sum_{n=1}^{3} a_{(n+5)_{xg}} (\Delta N_{sp})^n\end{aligned} \qquad (10)$$

where *x* and *g* represent the reaction type and energy group respectively, and $a_{j_{xg}}$ are Taylor series expansion coefficients.

In order to find the reducibility and correlation across the burnup range, the few-group homogenized macroscopic cross-sections of both Type 3c and Type 1 lattice in all reaction types and energy groups among all burnup steps are collected with the same arrangement, storing in $\mathbf{Y}_{Type3c}, \mathbf{Y}_{Type1} \in \mathbf{R}^{320\times 96}$ respectively. The loop sweeps as:

For each burnup step;
For each reaction type;
For each energy group.

The response matrix of multiple lattices $\mathbf{Y}_{Multiple} \in \mathbf{R}^{640\times 96}$ is the combination of $\mathbf{Y}_{Type3c}$ and $\mathbf{Y}_{Type1}$.

Apply RFA algorithm on uncertainties of both $\mathbf{Y}_{Type3c}$ and $\mathbf{Y}_{Multiple} \in \mathbf{R}^{640\times 96}$, results of the maximum error resulting from the dimensionality reduction and the rank, i.e. reduced dimension, used to reconstruct the model are depicted in Fig. 3. With a preset tolerance of relative error 0.1%, the uncertainty space of single lattice is reduced to $r = 20$, while of multiple lattices is reduced to $r = 23$. This indicates that the size of uncertainty space of few-group cross-sections can be significantly reduced to propagate the uncertainties, and introducing additional lattice types will only slightly increase the number of DOFs.

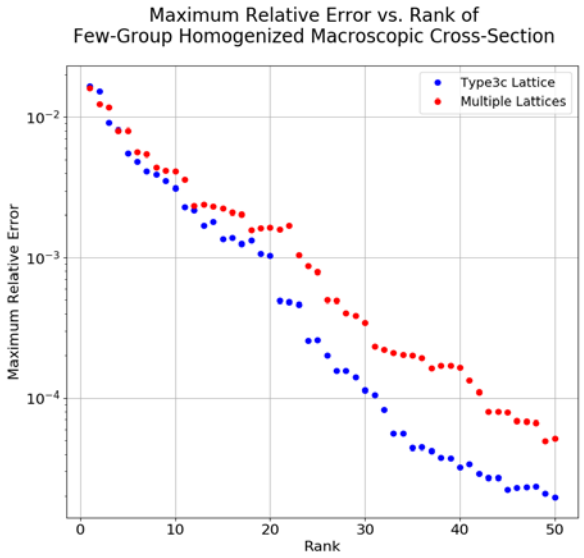

Fig. 3. Plot of error reduction vs. rank across depletions – all reaction types and energy groups included.

CONCLUSIONS

Uncertainty quantification is an indispensable analysis for nuclear reactor simulation as it provides a rigorous approach by which the credibility of the predictions can be assessed. This work has presented a ROM-based investigation on correlation structure and impact of multiple lattice models on uncertainty propagation in core calculation, implying that combination of multiple lattices in core simulation will not result in a significant increase of few-group cross-section uncertainty space. Future work will focus on functionalizing the few-group cross-section uncertainties in a compact form, amenable for storage and further manipulation by downstream core simulation.

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