Model Verification via Principal Component Analysis

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INTRODUCTION

Definitely, Verification and Validation (V&V) are the two most important practices by which the confidence in computational models is developed. However, the nature of the V&V practice implies that the analyst cannot decisively conclude that the model is an accurate representation within the region of interest.

Verification is the process of determining that a model accurately represents the conceptual description of the model and the governing equations and their solution. Validation is the process of determining the degree to which the model represents the natural phenomena. Therefore, V&V are vital to build the confidence that the model is correct or accurate for a specific scenario; thus, V&V cannot prove that a model is correct and accurate for all possible scenarios, but, rather, it can provide evidence that the model is sufficiently accurate for its intended use within a Region of Interest (RoI) [1].

Verification can be classified as code verification and solution verification. The purpose of code verification is to confirm that the software is working as intended. Therefore, code verification makes sure of the software quality assurance and to verify the correctness of the algorithms implemented therein. Code verification is partially accomplished using Software Quality Assurance (SQA), which is performed by the code developer and used to ensure that the code is implemented correctly and produces repeatable results on specified computer hardware, operating systems, and compilers. SQA is typically accomplished using configuration management and static and dynamic software quality testing [1]. Code verification also includes a process referred to as numerical algorithm verification where test problems with known (analytical) or highly fidelity (benchmark) solutions are devised and compared to solutions obtained with the code. However, in the absence of highly fidelity solutions, the method of manufactured solutions (MMS) can be used to create analytical solutions that are highly sensitive to algorithmic errors [1-3]. Moreover, verification can be applied to code analysis techniques such as the uncertainty quantification and sensitivity analysis. Note that no amount of verification is sufficient to make sure that a coded model is error-free. However, the accumulation of more and more of case studies provides an evidence help building the confidence of the computational model of interest.

It is natural in engineering communities to move from low fidelity models toward higher fidelity modeling and simulation techniques. An example of such effort can be illustrated by the Consortium for Advanced Simulation of Light Water Reactors (CASL) [4]. Such modeling effort definitely requires both validation and verification. However, many heavily validated and verified tools (with lower fidelity level) have been around for a long time such as the Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design [5]. If not utilized in the verification process such tools will be wasted!

While verification can help the analyst developing a statement on the performance of the model of interest, this statement is a stochastic statement and its precision depends on the number of samples used for the validation within the region of interest. There is almost no guarantee that any future sample will agree with the high fidelity model prediction! Therefore, in this summary the Principal Components Analysis (PCA) is used to check if the harmonics (modes, or degrees of freedom) predicted by the low fidelity model agree with what is considered a high fidelity model for the purpose of solution verification. Note that this summary does not concern the model verification (i.e. verifying whether the equations have been coded correctly), however, this work is concerned with verifying the solution of one simulator via comparison to the predictions of another high fidelity reference simulator or solution method (solution verification).

METHODOLOGY

This work introduces a model-to-model verification algorithm that arguably capable of establishing confidence in the harmonics produced by the high fidelity model predictions.

In order to represent the harmonics produced by both models, the Principal Component Analysis (PCI) will be employed. More specifically, the Singular Value Decomposition (SVD) is used to compute the singular values and the harmonics represented by the orthonormal bases [6-8].

In order to compute the harmonics from the two models involved in the study, the following steps are followed:

1. Sample the model parameter's sufficiently within a region of interest:
$$\boldsymbol{X} = [x_1 \dots x_k]$$
2. Run the model and collect the corresponding RoI (or vectors in the case of multivariate problem).
$$\mathbf{Y} = [y_1 \dots y_k]$$

3. Perform a rank revealing decomposition on the matrix **Y**. For example, the singular value decomposition (SVD) can calculate orthonormal basis of the subspace containing the variations (or snapshots) of the sensitivity coefficients:

$$\mathbf{Y} = \mathbf{USV^T}$$

where, **U** is the basis of the column space of the matrix **Y, S** is the singular values matrix and **V** is the matrix containing the basis of the row space of the matrix **Y**.

4. Based on the singular values (the diagonal of matrix **S**) determine the number of significant harmonics (dominant Degrees of Freedom-DoFs). This step will yield *r* DoFs.
5. Measure the angle between the two subspaces to determine the agreement of the harmonics generated by the low and high fidelity methods [9].

$$\sin(\vartheta) = \left\| \mathbf{U}_N \mathbf{U}_N^T - \mathbf{U}_C \mathbf{U}_C^T \right\|_2$$

Where, $\mathbf{U}_N$ is the basis of the basis of the lower fidelity subspace and $\mathbf{U}_C$ is the basis of the higher fidelity model or method.

SAMPLE CASE STUDY

In this section, a case study is picked to illustrate the algorithm presented in the previous section. This case study should not be viewed as a full and complete verification study. Rather, the purpose of this case study is to demonstrate and illustrate the proposed algorithm. Therefore, in this case study the performance of Course Mesh Finite Difference (CMFD) approximation and the Fine Mesh Finite Difference (FMFD) calculations of a depletion problem.

A reactivity-depletion problem will be used where the calculated the response of interest is the isotopic concentrations. This case study tried to compare the CMFD and the FMFD methods in terms of the harmonics by which the predicted concentrations are produced. The isotopic concentration predictability will be assessed via both methods where the FMFD calculations will be considered as the high fidelity source of data. While the CMFD calculations will be considered as the calculations to be verified.

One-quarter PLUS7 assembly was modeled using TRITON-NEWT (refer to Figure 1) to generate the burnup-dependent cross-section library, to be used by ORIGEN-ARP to obtain the isotopic concentration of the spent fuel at specific burnup (assembly average burnup in MWd/MTU) with a given initial fuel enrichment. In this study, fuel with the maximum enrichment is used in the depletion model (5%-w U-235) with no axial blankets or burnable absorbers. SCALE-6.1 standard materials are used for the radial gap gas (Helium), uranium dioxide (with 5%-w U-235) and water. Guide tubes and cladding are made of ZIRLO (Westinghouse ZIRLO).

The TRITON-NEWT uses ENDF-6 with 238 groups cross-section library. Each fuel pin is divided to 8 by 8 grid for the neutron transport calculations. It is a 2-D model with reflective boundary conditions to simulate the in-core conditions. General options and simulation parameters required by TRITON-NEWT are set to match recommended values in SCALE-6.1 Manual. The depletion problem followed the concentration of 240 isotope through the addnux=3 option available in TRITON sequence.

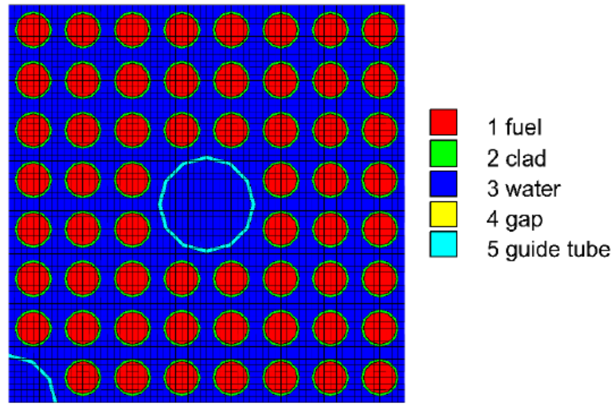

Figure 1. One quarter of PLUS7 assembly TRITON-NEWT model used for the depletion calculations.

In Figure **2**, the subspaces are constructed for each of the solution methods. For the CMFD, 1 course mesh was used. Note that the error tolerance used for this case study is the singular values, other resources use different techniques overviewed and developed in Ref. [7, 8]. Examining the figure below, 5 DoFs represent the data to a precision of 10^{-6} relative, therefore, *r*=5. However, this gives an idea about the number of important harmonics (the dimension of the subspace) and says nothing about the harmonics themselves. Therefore, in order to test the harmonics and whether they are the same, the angle test must be performed.

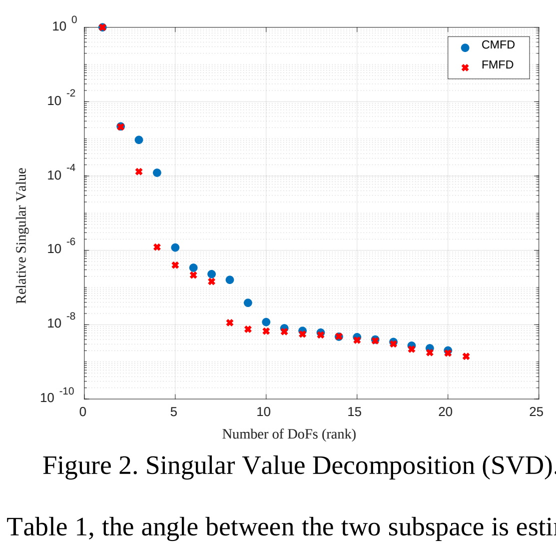

Figure 2. Singular Value Decomposition (SVD).

In Table 1, the angle between the two subspace is estimated. Note that first 1 one course mesh (CMs=1) is used where clearly the angle between the two subspaces is substantially large. Increasing the number of course meshes to 3 (CMs=3) the angle drops by one order of magnitude predicting a better agreement between the harmonics. This trend is further verified by the last test with 6 course meshes (CMs=6).

Table 1. Maximum Angle between the Two Subspaces.

	CMs=1	CMs=3	CMs=6
Maximum Angle (radians)	0.908	0.035	0.00001465

CONCLUSIONS

In this summary a new layer of verification is introduced and implemented via the proposed algorithm which tests if the two compared methods (model) not only produce predictions with statically compatible agreement but also there variations within the region of interest are along the same harmonics.

A depletion problem was used to illustrate the test the proposed algorithm. Note that the presented case study is not a complete verification analysis. The results indicated that the higher fidelity methods tends to agree better with the lower fidelity calculations, as more details are included.

Current and future works focuses on developing a more detailed algorithm with a physics based criteria to replace the singular values in the pursuit of the dominant DoFs.

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