# Physics-guided Neutronic Validation Methodology with Demonstration to KUCA cores

Siqi Zhang[1], Hany S. Abdel-Khalik[1,] Alberto Talamo[2] and Dimitri Rochman[3]

[1]School of Nuclear Engineering, Purdue University, 400 Central Drive, West Lafayette, IN 47906, USA
[2]Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA
[3]Paul Scherrer Institut, 5232 Villigen, Switzerland

## INTRODUCTION

Nuclear engineering field has some of the most stringent requirements for validation, heavily dependent on a comprehensive experimental campaign and guided by expert opinion in order to ensure proper coverage of the application domain conditions. With the increasing cost of experiments and the latest leaps in computer power, a new initiative has emerged promoting the use of high fidelity modeling and simulation to empower the validation process. The goal is to optimally combine the experimental and analysis results in a manner that reduces experts' subjectivity and minimize and preferably optimize the type and number of needed experiments.

Earlier work has introduced the concept of physics-guided validation as a science-driven approach to address some of the weaknesses of existing validation [1]. The developed method is denoted as physics-guided coverage mapping (PCM), which allows for mapping of experimental biases directly to the application domain. This summary applies the PCM methodology to the validation of MCNP to the simulation of the KUCA cores (Kyoto University Critical Assembly). It is assumed that only high-enriched KUCA core experimental data are available. PCM has two key steps, one employing a comprehensive uncertainty analysis to create a joint PDF that is used to characterize the applicability of the available experimental data to the prediction of low-enriched core behavior. This step will be done via the Total Monte Carlo (TMC) method [2]. The second step is predictive; it employs the constructed PDF to make predictions about the conditions of interest. This step will be completed using a nonparametric regression approach, denoted by the Alternating Conditional Estimation (ACE) [3].

## BACKGROUND

The primary challenge in any validation is to develop strong arguments to defend the use of simulation over the domain of application for which no or limited experimental data exist. The application domain refers to all the conditions/configurations that are envisaged for system operation, which may not be duplicated by experiments. This is because it could be either expensive or practically infeasible to conduct experiments for every condition expected during operation. To address that, a lot of experimental strategies are devised to provide credibility to model predictions for the wide range of conditions that form the application domain. This process is integral to any model validation exercise. Central to various methods for the model validation is the concept of scaling and mapping, that is how to translate the measured experimental biases into biases for the application conditions where no experimental values exist.

Taking the helicopter view, the state-of-the-art in model validation in the nuclear engineering community may be categorized into two general approaches. The first one, the calibration-based approach commences with the construction of detailed models for both the experimental and application domains and employs sophisticated mathematical theories to explain the discrepancy between measured and predicted responses via the adjustment of model parameters, typically physics parameters such as nuclear cross-sections and thermal-hydraulic parameters [4]. The adjusted parameters are then employed to predict the behavior of the system in the application domain. This approach has adopted many names according to the specifics of the mathematical theory employed, such as Bayesian calibration, generalized least-squares adjustment, or maximum likelihood estimation, See Refs [5-7] for examples. For a good review of calibration methods, see the seminal paper by Kennedy and O'Hagan [8].

The second approach is based on the concept of similarity, which refers to a quantitative metric that can be used to judge whether experiments are similar to the application conditions. This metric is a scalar quantity defined over a range, typically determined by experts. For example, for fluids calculations, the celebrated Reynolds number, representing a dimensionless ratio of inertial and viscous forces, is used to differentiate between laminar and turbulent flow and transition there between. In the neutronics' community, another metric is used which runs between zero and one, with one indicating perfect similarity and zero no similarity. The premise of this approach is that if high similarity can be established then the experimental biases are assumed to be representative of the biases to be expected in the application conditions. The biases are typically functionalized in terms of trending parameters, such as fuel-to-moderator ratio, fuel enrichment, etc., for neutronics, and wall roughness, flowrate, friction factors, etc., for fluid calculations, and the fit is used to predict the bias for the given application conditions [9]. When the similarity is low, additional uncertainties, referred to as scale-distortion uncertainties, are typically added on the

mapped biases to account for the dissimilarities between the experimental and application conditions [10]. The determination of the scale-distortion uncertainties is largely a subjective process as it is guided by expert-based analysis of the entire body of available experiments and analysis results to come up with appropriate uncertainties. The scale-distortion uncertainties are considered adequate when a group of independent experts agree to their validity.

For both of these approaches, if the mapped biases have unacceptably high uncertainties, new experiments are added, until an acceptable level of uncertainty is reached for the domain of application conditions. Both of these approaches suffer from unique challenges that are still considered unresolved. For detailed discussion, see an earlier publication [11].

## DESCRIPTION OF THE ACTUAL WORK

Central to this study is the use of PCM. A brief review is given herein. Let the physics model describing the experimental conditions and application domain be given by respectively

$$y_{\exp} = f_{\exp}(x,u) \quad (1)$$

$$y_{app} = f_{app}(x,v) \quad (2)$$

where $x$ are basic physics parameters, such as cross sections, which the two domains share the same values; $u$ and $v$ are control parameters that are unique to the experimental and application conditions, such as the materials, geometry and the composition specifications; $y_{\exp}$ are the experimental responses predicted by the model and $y_{app}$ are the responses of the application. Two responses can be of different types such as the flux, multiplication factor, and reaction rates.

PCM attempts to find a direct mapping between the experimental and the application domains. The mapping is obtained by using a joint probability distribution function (PDF) generated by performing a comprehensive uncertainty analysis of both the experimental and application conditions. The PCM algorithm proceeds as follows [1]:

1. Generate N samples of *x, u, v*
2. Execute the forward models for M experiments and applications N times, each with its corresponding samples. Their responses can be denoted by $y_{\exp}^{(i)}$ and $y_{app}^{(i)}$ respectively, where $i$ =1, 2…M. Let the measured value for each experiment be defined by $y_{\exp,msr}^{(i)}$, where $i$ =1, 2…M.
   These samples are used to construct an analytic joint PDF using kernel density estimation (KDE), see Ref. [10-11] for formal definition of KDE function.
3. Find a relationship between the response of the application $y_{\exp}^{(i)}$ and the experiments $y_{app}^{(i)}$ where $i$ =1, 2…M, and determine what the application response should be denoted by a vector $y_{proj}$. This variable is expected to be different from $y_{app}^{(i)}$ since not all the application can be covered by the experiments.
4. Using the measured experimental biases as input to the relationship developed in 3 and the PDF in 2, determine the estimated application bias, denoted $y_{proj,msr}$

The relationship in step 3 can be determined parametrically using response surface methods (see earlier publication [1]) or non-parametrically which is attempted in the current work. Specifically, we utilize alternating conditional estimation (ACE) algorithm which attempts to find an optimal transformation of the measured responses that best correlates with the application response of interest.

ACE was first introduced by Breiman and Friedman [3] for estimating the transformations of a response and a series of predictor variable in multiple regression that produce the maximum linear relationship between the transformed explanatory variables and transformed response variables. The optimal ACE transformations are solely derived from the given data and do not require a priori assumptions of any functional form for the response or predictor variables.

The ACE regression model has the general form:

$$\theta(y) = \alpha + \sum_{i=1}^{p} \phi_i(z_i) + \varepsilon \quad (3)$$

where $\theta$ is a function of the response variable, $y$ and $\phi_i$ are functions of $p$ predictors variables. Instead of estimating a linear function of a $p$-dimensional variable, the ACE attempts to uncover the non-linear feature by minimizing the unexplained variance of a linear relationship between the transformed response variable and the sum of the transformed predictor variables. See detailed discussion in [12-14]. In our implementation, we assume that there are $p$ experimental responses, each representing one of the predictor variables in Eq. (3), and $y$ represents the response in the application domain, where no experimental data exists. Following step #2 of the PCM algorithm, samples from the PDF are used to train the ACE model in Eq. (3):

$$y_{proj}^{ACE} = \theta^{-1}\left(\alpha + \sum_{i=1}^{p} \phi_i(z_i) + \varepsilon\right)$$

where $z_i$ are sampled from the PCM-generated joint PDF. After training, the measured values for the responses are used to perform a prediction step as follows:

$$y_{proj,msr}^{ACE} = \theta^{-1}\left(\alpha + \sum_{i=1}^{p} \phi_i(z_i^{msr}) + \varepsilon\right)$$

Returning back to Eqs. (1) and (2), the shared physical parameters $x$ representing the common sources of uncertainties are the nuclear cross sections. The uncertainty analysis is completed using N=338 random samples of the nuclear data libraries, generated using the nuclear data uncertainty stochastic sampling method (NUSS) [2,15]. The NUSS is a new stochastic-sampling based tool which combines the efficiency of multi-group uncertainties and the

transparency of point-wise energy nuclear data. It employs perturbations to the point-wise nuclear data given in the ACE format using the multi-group nuclear data covariance. The specific ACE format can be directly transferred to MCNP for criticality safety and burnup calculations.

The sampling of nuclear data in NUSS method follows the methodology by Wieselquist [16]. Group-wise perturbation factors as the ratio between the sampled and nominal group-wise nuclear data are employed to the point-wise nuclear data in the ACE format. The NUSS module to modify the original ACE format separates the entire length of the nuclear data into G groups, which is the number of the energy groups in the given covariance library. The covariance files of ENDF/B-VII.1 are processed in 187 groups and used to generate the random cross section groups. The following nuclear data can randomly be modified at once: $\bar{\nu}$ (emitted neutron per fission), $\chi$ at different neutron incident energy (prompt fission neutron spectra), and cross sections for (n, tot), (n, el), (n, inl), (n, 2n), (n, f) and (n, c). Only the isotopes of $^{235}$U and $^{238}$U are varied, which are the main sources of the uncertainties for k-eff calculations.

## NUMERICAL RESULTS

A demonstrative numerical experiment employs the KUCA cores with high and low enriched uranium fuel pins, denoted by HEU and LEU, respectively. The HEU U-Al alloy-based core (93% uranium enrichment) is selected to represent the experiment and the application is the LEU U-Al alloy with only 19.75% uranium enrichment. The number densities of these two fuels are shown in the table 1.

Table 1. Number densities of HEU and LEU

| HEU U-Al | | LEU U-Al | |
|---|---|---|---|
| $^{235}$U | 1.50694E-03 | $^{235}$U | 3.19061E-04 |
| $^{238}$U | 1.08560E-04 | $^{238}$U | 1.29644E-03 |
| $^{27}$Al | 5.56436E-02 | $^{27}$Al | 5.56436E-02 |
| Total | 5.72591E-02 | Total | 5.72591E-02 |

Calculations are performed using MCNP6 with the 336 NUSS-generated ACE libraries. The employed MCNP models are based on an earlier study [17], with the fuel assembly shown schematically in Fig. 1.

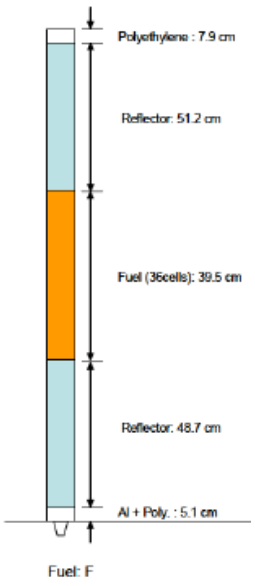
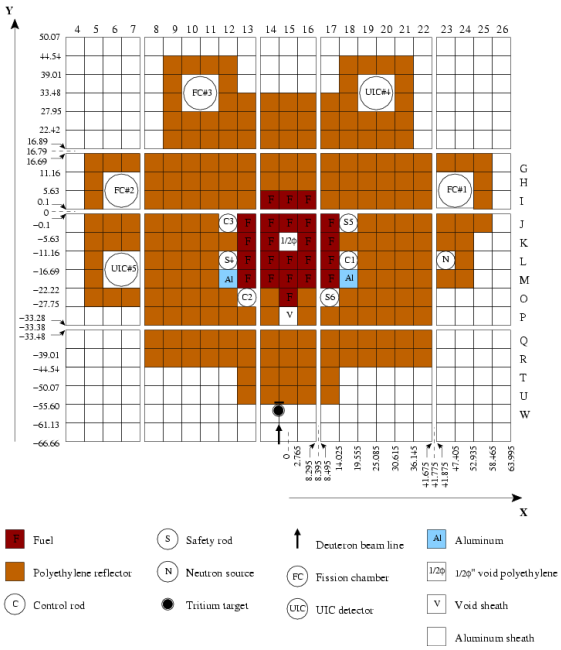
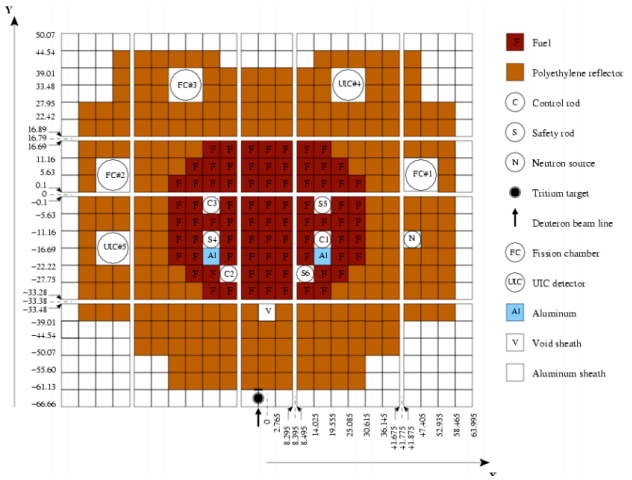



Figure 1. The description of Fuel F

The fuel assembly with U-Al alloy is filled in the middle with reflector polyethylene on both sides. And the fuel regions in the KUCA core are obtained by the stacking plates. The whole core configuration [17] for which numerical calculations have been performed is shown in Fig. 2. The configuration of LEU is a little different from that of HEU. The additional fuel assemblies around the center of the core are required to make the low-enriched KUCA core critical.




(a) HEU configuration




(b) LEU configuration

Figure 2. The KUCA core configuration
"Source: Ref [17]"

For this numerical experiment, both k-eff and the group flux (at location (K,15) and (H,19), denoted by points O and A, respectively) are used as representative responses in the experimental and application domains. PCM allows one explore all possible correlations between the responses in the experimental and application domain to allow for a quantitative approach by which the value of the experiment can be measured. For example, Fig. 3 shows the k-eff PCM-generated joint PDF between the HEU and LEU (both axes are centered around their mean values), the standard correlation coefficient is calculated to be 0.961905. Figs. 4(a) and 4(b) show the correlations between the HEU and LEU for different energy ranges at the same spatial location, point O. Specifically, Fig. 4(a) shows the thermal-to-thermal flux correlations in the energy range ($10^{-4}$ eV to 1eV), while Fig. 4(b) shows the fast correlations in the range (1eV to 100MeV). The standard correlations calculated for the two cases are, respectively, 0.696862 and 0.852418.

Spatial correlations can also be explored, see for example the joint PDF between the thermal fluxes at points O and A. The standard correlation coefficient for this case is 0.708168. Comparison of these results may be used to judge the value of spatial and energy correlations in mapping biases between experimental and application domain.

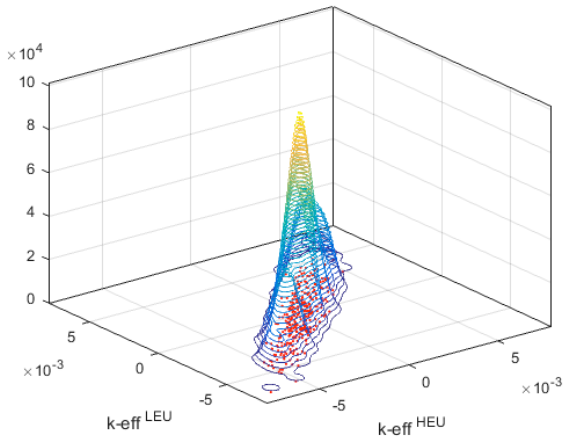
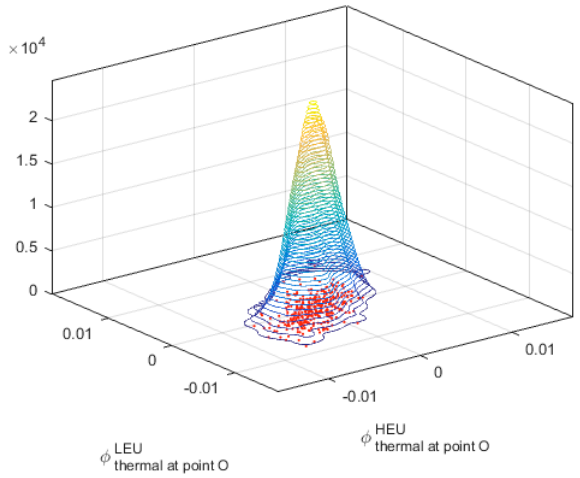
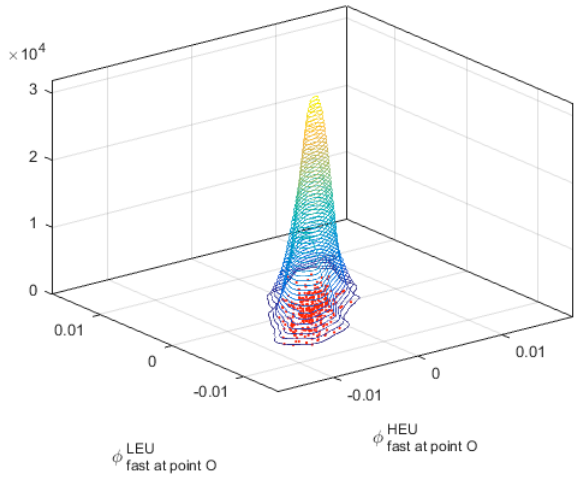



Figure 3. (HEU, LEU) k-eff joint PDF




(a) Thermal group




(b) Fast group

Figure 4. (HEU, LEU) 2-group flux joint PDF

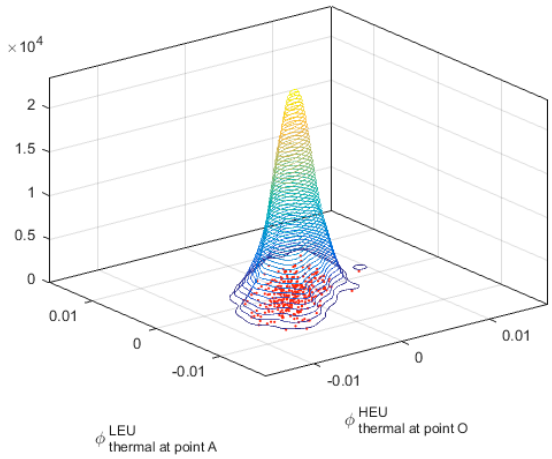
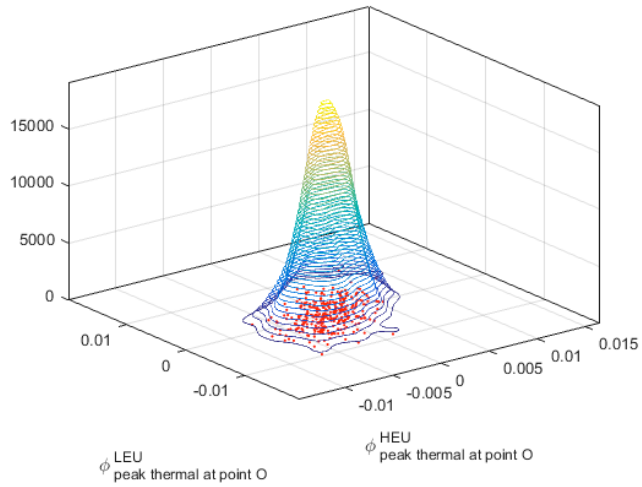



Figure 5. (HEU, LEU) thermal flux joint PDF at position A and O

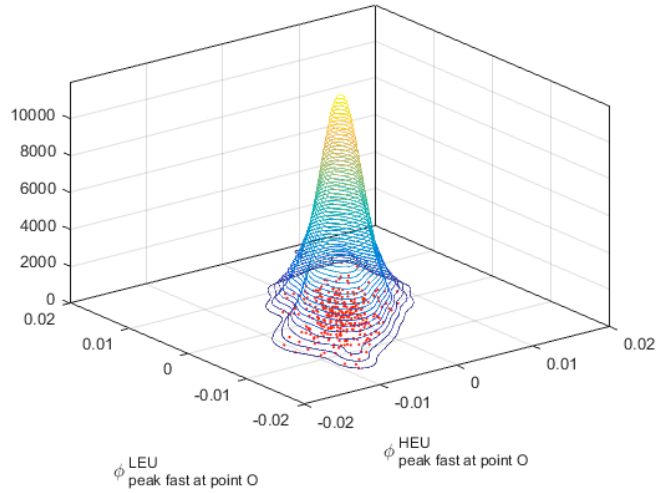
The utility of the above PDFs is very intuitive as they directly relate the response of interest to the experimental response by taking into account the variability of both responses due to uncertainties, i.e., $p\left(y_{\exp}, y_{app}\right)$. Currently, we are only taking into account cross-section uncertainty. The idea however can be easily extended to account for other sources of uncertainties, such as modeling and numerical errors, and uncertainties resulting from technological parameters such as dimensions, composition, etc. With the experimental data available, in the form of a PDF $p\left(y_{\exp}\right)$, one can marginalize the joint PDF using the experimental data to calculate the PDF for the response of interest as follows:

$$p\left(y_{app}\right) = \int p\left(y_{\exp}, y_{app}\right) p\left(y_{\exp}\right) dy_{\exp}$$

PCM can also allow one explore the value of using more refined models for the experiment and/or application. For example, one could explore the value of using more groups to analyze the flux variations. For illustration, a 53 group model is used for both the LEU and HEU models. Fig. 6 shows the peak group-to-peak group correlations in both the thermal and fast ranges for the HEU and LEU, with calculated standard correlation coefficients of, respectively, 0.569956 and 0.718097. The results show that the correlations are decreased by about 10% from the values calculated in Fig. 4. The implication is that one can use these simple analysis results to judge the value of model investments without having to rely on complicated mathematical techniques. Further, more elaborate weighting approaches combining both spatial and energy-dependent fluxes can be devised to maximize correlations with the application response of interest.




(a) Thermal group




(b) Fast group

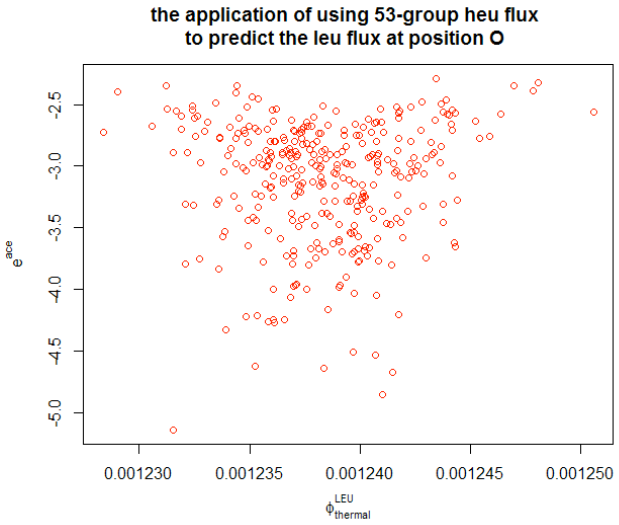
Figure 6. (HEU, LEU) 2-group peak flux joint PDF

The results shown so far are meant for illustration purposes only as they communicate to the analyst the value of each individual experimental value to the application response of interest. In reality, an analytic approach must be devised to combine all available experimental data to maximize inference of the response of interest. This manuscript demonstrates the use of the ACE algorithm to combine experimental data in a non-parametric approach. In this approach, each experimental response is treated as a predictor variable, and the algorithm attempts to find the best non-parametric relationship between the experimental responses and the application response of interest.

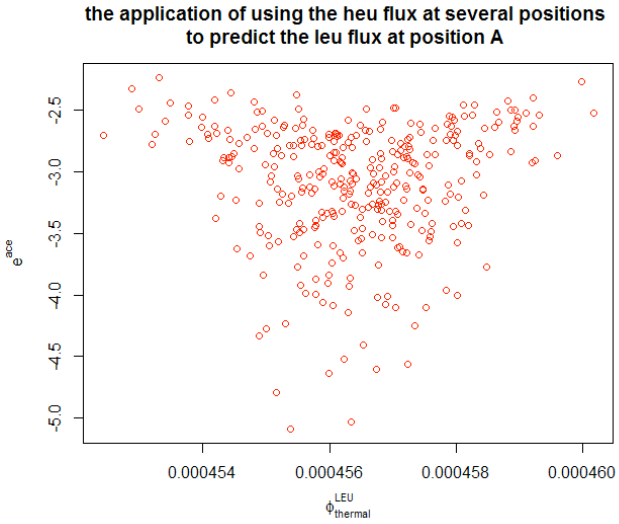
Two ACE experiments are performed to find the possible relationship between LEU and HEU KUCA cores. The objective of both tests is to estimate the response in the application domain by all available experimental data. The first test employs 53-group flux data for HEU at location O as the experimental data and the 2G thermal flux for LEU at

the same location as the response. The second test attempts to describe the group-wise flux at certain position with the experimental group-wise flux data from other positions.

Figure 7 shows the reconstructed error by the ACE transformation. The x-axis describes the absolute value of the fluxes, and the y-axis represents the log-10 of the error in relative units. Both plots show that the relative errors are uniform regardless of the nominal value of the flux.




(a) Test 1




(b) Test 2

Figure 7. Reconstructed error by ACE of the application responses

## CONCLUSION

This summary explores the application of a recently-developed physics-guided approach denoted by PCM to support the validation of using MCNP for the analysis of the KUCA cores. We investigate the relation of the biases and uncertainties between the highly-enriched fuel pins and low-enriched fuel pins and attempt to find the mapping that describe their mathematical transformation. The numerical results notice a fairly linear correlation for the reactivity, thermal flux and fast flux between HEU and LEU. Also, the ACE tests are performed to find the maximum linear effect between the HEU and LEU. For the further work, we want to proceed more detailed discussion about the non-parametric statistical analysis to describe the application response more accurately.

## REFERENCES


1. H.S. Abdel-Khalik, A. I. Hawari, and C. Wang. "Physics-guided Covered Mapping: a new approach for quantifying experimental coverage and bias scaling." Transcations of the American Nuclear Society112 (2015): 704-707.
2. D. Rochman, A. Vasiliev, H. Ferroukhi, T. Zhu, S. C. van der Marck, and A. J. Koning. "Nuclear data uncertainty for criticality-safety: Monte Carlo vs. linear perturbation." Annals of Nuclear Energy 92 (2016): 150-160.
3. L. Breiman, and Jerome H. Friedman. "Estimating optimal transformations for multiple regression and correlation." Journal of the American statistical Association 80, no. 391 (1985): 580-598.
4. Gandini, M. Petilli, "AMARA: A Code Using the Lagrange Multipliers Methods of Nuclear Data Adjustment," RT/FI(73)39, Comitato Nazionale per l'Energia Nucleare, (1973).
5. G. Palmiotti, M. Salvatores, M. Aliberti, H. Hiruta, R. McKnight, P. Oblozinsky, and W. S. Yang, "A global approach to the physics validation of simulation codes for future nuclear systems." Annals of Nuclear Energy 36.3 (2009): 355-361.
6. D.G. Cacuci, and M. Ionescu-Bujor. "A comparative review of sensitivity and uncertainty analysis of large-scale systems-II: Statistical methods." Nuclear Science and Engineering 147, no. 3 (2004): 204-217.
7. M. Jessee, H. Abdel-Khalik, and P. Turinsky. "Evaluation of BWR Core Attribute Uncertainties due to Multi-group Cross-Section Uncertainties."Proc. of M&C (2007).
8. M.C. Kennedy and A. O'Hagan. "Bayesian calibration of computer models." Journal of the Royal Statistical Society: Series B (Statistical Methodology) 63, no. 3 (2001): 425-464.
9. B. L. Broadhead, C. M. Hopper, R. L. Childs, and C. V. Parks. "Sensitivity and uncertainty analyses applied to criticality safety validation." NUREG0CR-6655, Vols 1 (1999).
10. B.E. Boyack, I. Catton, R. B. Duffey, K. R. Katsma, G. S. Lellouche, S. Levy, G. E. Wilson, and N. Zuber. "Quantifying reactor safety margins part 1: an overview of the code scaling, applicability, and uncertainty evaluation

methodology." *Nuclear Engineering and Design* 119, no. 1 (1990): 1-15.
11. D. Huang, H.S. Abdelk-Khalik, "Construction of Optimized Experimental Responses in Support of Model Validation via Pyhsics Coverage Mapping Methodology." *PHYSOR Meeting*, Sun Valley, ID, 2016
12. E. Parzen, "On estimation of a probability density function and mode." *The annals of mathematical statistics* 33, no. 3 (1962): 1065-1076.
13. V. A. Epanechnikov, "Non-parametric estimation of a multivariate probability density." *Theory of Probability & Its Applications* 14, no. 1 (1969): 153-158.
14. D. Wang, and Michael Murphy. "Estimating optimal transformations for multiple regression using the ACE algorithm." *Journal of Data Science* 2, no. 4 (2004): 329-346.
15. T. Zhu, "Sampling-Based Nuclear Data Uncertainty Quantification for Continuous Energy Monte Carlo Codes." PhD diss., ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE, 2015.
16. W. Wieselquist, T. Zhu, A. Vasiliev, and H. Ferroukhi. "PSI methodologies for nuclear data uncertainty propagation with CASMO-5M and MCNPX: Results for OECD/NEA UAM benchmark Phase I." *Science and Technology of Nuclear Installations* 2013 (2013).
17. G. Aliberti, J. A. Morman, J. G. Stevens, J. Roglans-Ribas, “Analysis of the KUCA Type-A Experiments”. *Argonne National Laboratory project report* ANS/GTRI/TM-14/2