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Raleigh, North Carolina, USA, November 13th, 2023

To: Science Council, National Centre for Nuclear Research

Assessment of the Doctoral dissertation by Mr. Michał Jędrzejczyk
"Establishment of best practices in reducing uncertainties in multigroup cross-sections with Bayesian methods"

This doctoral thesis investigated and implemented Sequential Monte Carlo – Approximate Bayesian Computation (SMC-ABC) method to reduce the keff uncertainty, and compares it to two other approaches, namely Generalized Linear Least Squares (GLLS) and a General Monte Carlo-Bayes Procedure for Enhanced Predictions of Integral Functions of Nuclear Data (MOCABA). The major part of the performed work is evaluation of these three methods based on their performance in calibrating neutron cross-sections using experimental data from the ICSBEP Handbook. Furthermore, two novel concepts for inverse problems of nuclear engineering have been introduced: validation using synthetic cross-sections and analysis of the influence of uncalibrated cross-sections on the calibration results. Finally, this thesis also established a few best practice guidelines in reducing uncertainties in multi-group cross-sections with Bayesian methods, which are important for nuclear reactor design and safety analysis. This thesis is overall well-written, with most concepts clearly explained, and the presented results are supportive of the major findings.

Reduction of the uncertainties in neutron cross-sections has been a long concern for nuclear reactor physics analysis. This is because the neutron cross-sections are essential for calculating the criticality factor (keff) that determines the reactor's power level and safety margin, as well as simulating the neutron transport and fission processes in existing and advanced nuclear reactors. Even though inverse uncertainty quantification and Bayesian calibration have been widely studied in the nuclear thermal-hydraulics area, the application and developed of Bayesian-based approaches are under-studied. Therefore, a PhD thesis on establishing best practices in reducing uncertainties in multi-group cross-sections with Bayesian methods is a timely and relevant topic that can contribute to advancing the nuclear energy sector and addressing its challenges. This is exactly what has been offered by this doctoral thesis. The provided best practice guidelines in reducing uncertainties in multi-group cross-sections with Bayesian methods can be very useful for nuclear data evaluation and nuclear reactor safety analysis with reduced uncertainty.

The PhD thesis has several original and innovative contributions. First of all, the comprehensive comparison of GLLS, MOCABA and SMC-ABC based on an ICSBEP benchmark is very useful to the nuclear community to understand the merits and limitations of each method. Secondly, it introduces two novel concepts in the field of nuclear engineering inverse problems: validation using synthetic cross-sections and analysis of the influence of uncalibrated cross-sections on the calibration results. The thesis shows that SMC-ABC is a universal and rigorous method that can produce any posterior distribution and handle non-linear models, but it requires significantly more computational power than GLLS and MOCABA, which are limited

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to multivariate normal distributions and linear models. The thesis demonstrates that validation using synthetic cross-sections can verify whether the posterior cross-sections are closer to their true values, and that neglecting the uncertainties and correlations of uncalibrated cross-sections can lead to serious underestimation of the posterior uncertainty of the calibrated cross-sections.

This doctoral thesis is 120 pages long with 6 chapters. There is also a reference section but no appendices. The outline has been properly generated with a list of figures, a list of tables, nomenclatures, author's contribution and abstract. The bibliography consists of 50 references that cover a wide span of literature, which shows the author's good orientation in the research topic. A reasonable number of figures, tables, and equations have been included and they are properly referred to in the main body of the thesis.

The general outline of this doctoral thesis is appropriate. Chapter 1introduces the topic of the thesis, as well as its objective and scope. Chapter 2 provides the details of three Bayesian calibration algorithms, GLLS, MOCABA and SMC-ABC. Chapter 3 describes the software and data used for simulating criticality safety of nuclear systems, namely SCALE, CSAS5, CENTRM, and TSUNAMI modules, and the ENDF/B-VII cross-section library. Chapter 4 presents a comparison of three Bayesian calibration algorithms: GLLS, MOCABA, and SMC-ABC, applied to reduce uncertainty in 56-group U-235 cross-sections for fast systems. Chapter 5 applies the MOCABA algorithm to calibrate 1904 neutron cross-sections relevant to HTGRs using 34 experiments from the ICSBEP handbook. Chapter 6 proposes a best-practices algorithm for reliable calibration of neutron cross-sections using Bayesian methods and experimental data.

Compared to nuclear thermal-hydraulics, neutronics simulation is a less studied area using Bayesian-based approaches, especially for forward and inverse uncertainty quantification. Therefore, this thesis fills this gap by the three major contributions: (1) comparison of GLLS, MOCABA and SMC-ABC based on an ICSBEP benchmark, (2) validation using synthetic cross-sections and analysis of the influence of uncalibrated cross-sections on the calibration results, and (3) best practice guidelines in reducing uncertainties in multi-group cross-sections with Bayesian methods. The major contributions are presented in Chapters 4, 5 and 6. This thesis is well-written in general, with a clear outline and presentation. The reasoning is well defined and consistent, and the conclusions are well supported by the presented results. The results obtained are undoubtedly crucial for the further development and validation of codes for simulating nuclear installations.

One major criticism of this thesis is the presentation of the SMC-ABC algorithm in Section 2.3. As the implementation of SMC-ABC is considered a major contribution of this thesis, sufficient details about this algorithm should be provided. Section 2.3 only has one equation and it is much shorter than Section 2.1 and 2.2 on GLLS and MOCABA. Also, Figure 2 and Algorithm 1 are both adapted from existing publications. The author is suggested to provide a more comprehensive introduction to this new algorithm, using more illustrative tools (figures, diagrams, flowcharts, etc.) to make it easier to understand.

Another potential improvement is about the References. 50 papers in a doctoral thesis are generally too few, even though they cover a wide span of the literature relevant to the performed work (mostly neutronics simulations), as mentioned earlier. Chapter 1 should include a more comprehensive literature survey on inverse UQ in nuclear engineering, Bayesian calibration in nuclear engineering, non-Bayesian based uncertainty reduction approaches in neutronics simulations, ABC application in other areas. There are many references on ABC applications, which should be covered in the literature survey.

Below is a list of some suggested editorial revisions:

1. In the “List of Tables”, when a table spans two pages, two items are included in the List with the same title. This does not seem necessary.
2. Page 15, the author’s contribution description seems too short, it should be significantly expanded.
3. For figures taken from References such as the ICSBEP Benchmark, proper references should be provided in the figure captions, for example, Figures 20, 21, 22, etc.
4. Page 20, title of Section 1.1 “IV generation nuclear reactors”. People always just call them “Generative IV” or “Gen. IV”.
5. Figure 1: resolution is too low. It looks like a snapshot from a presentation because the lower right corner has a number "15".
6. Figure 1: caption, fix "...of IV generations...", "Gen. IV" is not "IV generations." Also, these six acronyms have already been defined previously.
7. Page 26, "...supported by a polynomial surrogate model for...", Reference [19] used Gaussian Process-based surrogate models, instead of polynomials. More details are included in the reference “*Wu, X., Kozlowski, T., Meidani, H., & Shirvan, K. (2018). Inverse uncertainty quantification using the modular Bayesian approach based on Gaussian Process, Part 2: Application to TRACE. Nuclear Engineering and Design, 335, 417-431*.” Please consider adding this reference.
8. Page 27, "The publications [28] and [29] use the SMC-ABC method to..." are these two references only used ABC, or SMC-ABC?
9. Page 41, "PyMC implementations [41] and [42]", these two references may be improved. Is "10.5281/zenodo.5654871" the doi or supposed to be a link?
10. Chapter 3, Page 45 - page 51, does not include any references. But multiple papers should be referenced in this section, especially those for SCALE, ENDF, and the various modules mentioned.
11. Page 111, "Algorithm 4 Step-by-step instruction on how to successfully calibrate neutron cross-sections," - This is not really an algorithm. Can simply use a diagram with details presented in a list of steps. An algorithm should be concise and presented with math symbols.

After reviewing this dissertation, I believe that it meets all the customary and legal requirements for a PhD thesis. Therefore, I request that Mr. Michał Jędrzejczyk be admitted to the public defense and further stages of the doctoral dissertation.

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