Programme doctoral en – *Doctoral Program in*
ENERGIE – *ENERGY*

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

RAPPORT ANNUEL DE THESE [2013]

Annual Thesis Report [2013]

Development and Assessment of Nuclear Data Uncertainty Propagation Methodologies for Criticality Safety Calculations with Monte Carlo Codes

Nom du/de la candidat(e) / *Name of the candidate* : Ting ZHU ....

Non du directeur de thèse / *Name of thesis director* : Prof. Dr. Andreas Pautz ....

Date d'examen de candidature / *Candidacy exam date :* 05.04.2012 ....

Signatures :

Candidat(e) / *Candidate* : ....

Directeur de thèse / *Thesis director* : ....

Directeur du Programme doctoral/*Director of doctoral program* : ....

Date : ....

Un exemplaire de ce rapport annuel ainsi que la lettre d'appréciation du Directeur de thèse doivent être adressés, après signatures par le Directeur de thèse et le Candidat, à la Direction du Programme Doctoral en Energie EDEY/ME B1 344/Station 9/1015 Lausanne, chaque fin d'année entre décembre et début mars.

One copy of this yearly thesis report as well as an appraisal letter by the thesis director must be sent to the direction of the doctoral program in Energy, EDEY/ME-B1 344/Station 9/1015 Lausanne, duly signed by the Candidate and the Thesis Director, every year end between December and beginning of March.

RAPPORT / *Report*

1) **Objectifs du travail (5 à 10 lignes) /** *Objectives of the research (5 to 10 lines)*

The purpose of the research is to develop a stochastic sampling methodology for nuclear data uncertainty propagation in the frame work of criticality safety assessment at LRS/PSI. Nuclear data uncertainty propagation capabilities are to be implemented for particle transport code MCNP(X) and the continuous nuclear data used by MCNP(X). In criticality safety calculation, the ability to separate nuclear data uncertainties from other sources of uncertainties in k_{eff} will allow LRS/PSI to update the Swiss criticality safety methodology.

2) **Travaux accomplis durant l'année écoulée (état de la problématique) /** *Work achieved during the past year (state of research)*

The NUSS (Nuclear data Uncertainty Stochastic Sampling) tool for the sampling and propagation of nuclear data was verified against the deterministic-based TSUNAMI code by ORNL and another stochastic-sampling-based Total Monte Carlo (TMC) method by NRG. The results of comparison showed good agreement between NUSS and TSUNAMI, but the ^{239}Pu(υ-bar) uncertainty contribution in Jezebel (bare plutonium sphere critical benchmark) differed the most between NUSS and TMC approach. Furthermore, capability to build flexible energy-group structures for covariance data by the nuclear data processing code NJOY enables preliminary assessment on the k_{eff} uncertainty discrepancies due to covariance library differences. For example, significant differences in the ^{239}Pu(υ-bar) covariance data were found between the ENDF/B-VII.1 and SCALE6-44g covariance libraries such that in Burnup calculations of the UAM pincell benchmarks (Phase-Ib), the total k_{eff} uncertainty can have the opposite time-dependent behavior due to the production of ^{239}Pu in the depletion calculation [1].

An updated version of NUSS (called NUSS-RF) has been implemented in order to estimate the individual contribution of nuclear data uncertainty simultaneously while keeping the merits of the stochastic sampling approach. NUSS-RF uses Random Balance Design (RBD) method to sample nuclear data such that the calculation of individual input variance is achieved by the Fourier Amplitude Sensitivity Testing (FAST) algorithm. This combined procedure is able to overcome the typical challenges in nuclear data uncertainty quantification, which are predominantly the large number of nuclear data inputs and the correlations among them. NUSS-RF is applied to Jezebel, Godiva fast benchmarks, as well as a BWR pin-cell model (from UAM Phase I). In all three cases, NUSS-RF and deterministic Sensitivity/Uncertainty (S/U "sandwich rule") approach have good agreement on the magnitude and ranking of the top uncertainty contributors by their variance fractions when the input parameters are independent. In case of correlated inputs, the level of correlation impacts the agreement between the two methods, in both the magnitude and ranking of input variance fractions. It is found that in NUSS-RF method, a strong correlation among inputs tends to result in similar variance fractions (or importance) in the same inputs, whereas such effect is not observed in the results by the S/U approach.

3) Etat d'avancement / *Current state of work*

Further development of the NUSS-RF method will focus on optimizing the RBD sampling and FAST variance calculation schemes (e.g. sample sizes and harmonics order), as well as the determination of higher order Sensitivity Indices. In addition, a rigorous and quantitative interpretation of the variance fraction for correlated inputs is of great interest for establishing the relation between NUSS-RF and S/U approaches (ie. Global vs. Local Sensitivity Analysis). The NUSS-RF method should also be tested for benchmarks where the uncertainty of individual isotope-reaction (as opposed to the single energy-dependent reaction in this work) can be determined and ranked.

The NUSS-RF method is to be applied to LRS/PSI's validation set of benchmarks to assess k_{eff} uncertainty due to nuclear data uncertainties for criticality safety evaluation methodology. This task involves recalculating the 149 benchmarks within the validation set, each of which is run many times (on the order of hundreds) to obtain both the total k_{eff} uncertainty and a breakdown of the individual nuclear data uncertainty contributions. The aim is to update the current PSI Criticality Safety Assessment methodology which has only considered uncertainties in the k_{eff} bias due to modelling and experimental uncertainties.

4) Calendrier des travaux à venir / *Calendar of upcoming work*

Time Frame	Task Description	Publication
March – April 2014	Refinement on NUSS-RF Recalculation of benchmark validation set with NUSS-RF Thesis writing	Thesis draft review by Chapters: Methodology, Literature Review
April – May 2014	Thesis writing Participate in *Annual NES PhD Day*	Thesis draft review by Chapters: Verification/Validation/Applications, Introduction
June – July 2014	Thesis writing and revision Participate in *International Youth Nuclear Congress*	Thesis complete draft submission (including Conclusion, Future Works)
August – Oct. 2014	Thesis defense (Closed) Thesis defense (Open) Prepare 4th Journal paper on Global Sensitivity Analysis and NUSS-RF Participate in *PHYSOR 2014*	4th Journal contribution on Global Sensitivity Analysis and NUSS-RF (draft) PSI Memo/AN/TM on proposals for CSE methodology refinements

5) Publications scientifiques, exposés, conférences ou séminaires présentés par le candidat /

Scientific publications, presentations, conferences or seminars held by the candidate

1) **T. Zhu**, D. Rochman, A. Vasiliev, H. Ferroukhi, W. Wieselquist and A. Pautz, *Comparison of Two Approaches for Nuclear Data Uncertainty Propagation in MCNP(X) for Selected Fast Spectrum Critical Benchmarks* , **Nuclear Data Sheets,**2014 **(accepted)**

2) **T. Zhu**, A. Vasiliev, H. Ferroukhi and A. Pautz, *Application of the PSI-NUSS Tool for the Estimation of Nuclear Data Related* k_{eff} *Uncertainties for the OECD/NEA WPNCS UACSA Phase I Benchmark*, **Nuclear Data Sheets**, 2014 **(accepted)**

3) **T. Zhu**, *NUSS Tool for Nuclear Data Uncertainty Quantification Using Stochastic Sampling Approach,* **PSI NES PhD Student Day Presentation**, May 2013

4) **T. Zhu**, A. Vasiliev, H. Ferroukhi and A. Pautz, *NUSS: A Tool for Propagating Multigroup Nuclear Data Covariances in Pointwise ACE-Formatted Nuclear Data Using Stochastic Sampling Method*, **Journal paper (under internal review)**

5) **T. Zhu**, A. Vasiliev, H. Ferroukhi, A. Pautz and S. Tarantola (JRC), *NUSS-RF: Stochastic Sampling-Based Tool for Nuclear Data Sensitivity and Uncertainty Quantification,* **PHYSOR 2014 Conference**, Sept. – Oct. 2014, Kyoto Japan **(submitted)**

6) **T. Zhu**, A. Vasiliev, H. Ferroukhi and A. Pautz, *Stochastic Sampling-Based Tool for Nuclear Data Sensitivity Uncertainty Quantification*, **International Youth Nuclear Congress,** July 6-12, 2014, Burgos, Spain (**accepted**)

References

[1] H. J. Park, H. J. Shim and C. H. Kim, *Uncertainty Propagation Analysis for PWR Burnup Pin-Cell Benchmark by Monte Carlo Code McCARD*, Science and Technology of Nuclear Installations, Vol. 2012, Article ID 616253

Directives pour rapports annuels de thèse
Directives for yearly thesis reports

Page de couverture

Elle comportera les informations suivantes :

- Titre de la thèse
- Caractère du rapport (annuel, final)
- Date d'immatriculation
- Date d'admission à la thèse
- Directeur de thèse
- Candidat
- Directeur du programme doctoral
- Date du rapport

Cover page

Please indicate the following data :

- *Thesis title*
- *Kind of report (annual, final)*
- *Date of immatriculation*
- *Date of thesis admission*
- *Thesis director*
- *Candidate*
- *Director of doctoral program*
- *Date of report*

Corps du rapport

Il présentera les rubriques suivantes :

- Objectifs du travail (5 à 10 lignes)
- Travaux accomplis durant l'année écoulée, état de la problématique
- Etat d'avancement
- Calendrier des travaux à venir
- Publications scientifiques
- Exposés, conférences ou séminaires présentés par le candidat

Body of report

Present the following information :

- *Work objectives (5 to 10 lines)*
- *Work achieved during the past year, state of the research*
- *Current state of work*
- *Calendar of upcoming work*
- *Scientific publications*
- *Presentations, conferences or seminars held by the candidate*

Au total, entre 3 à 5 pages /
In total, between 3 and 5 pages

EDEY/ Dec. 2011