International Workshop of Nuclear Data Covariances

Program and Book of Abstracts

Local Organizing Committee
D. Neudecker, T. Kawano, P. Talou and M.B. Chadwick

LA-UR-14-21549

Program

Monday, April 28, 2014

8:00-9:00	Registration Desk
9:00-9:20	Welcome
Section	Introduction & Worldwide Nuclear Data Libraries and Related UQ Efforts
Chair	M. Herman
9:20-9:50	D.L. Smith
9:50-10:20	R. Capote
10:20-10:50	Coffee Break
Section	Worldwide Nuclear Data Libraries and Related UQ Efforts
Chair	M.B. Chadwick
10:50-11:20	M. Herman
11:20-11:45	R. Xu
11:45-12:15	S. Ganesan
12:15-12:45	A.D. Carlson
12:45-14:15	Lunch Break
Section	Formatting, Benchmarking and Target Accuracies
Chair	M. Salvatores
14:15-14:45	C. Mattoon
14:45-15:15	G. Palmiotti
15:15-15:40	S. Hoblit
15:40-16:10	Coffee Break
Section	Benchmarking and Target Accuracies
Chair	P. Griffin
16:10-16:35	M.E. Dunn
16:35-17:00	B.A. Khuwaileh
17:00-17:25	G. Chiba

Tuesday, April 29, 2014

Section	Reactor Applications
Chair	G. Palmiotti
9:00-9:30	M. Salvatores
9:30-9:55	G. Aliberti
9:55-10:20	C. Diez
10:20-10:50	Coffee Break
Section	Reactor Applications
Chair	M.E. Dunn
10:50-11:20	J.-Ch. Sublet
11:20-11:45	G. Arbanas
11:45-12:10	M.L. Williams
12:10-12:40	K. Yokoyama
12:40-14:10	Lunch Break
Section	Applications and Transport Calculations
Chair	J.-Ch. Sublet
14:10-14:40	B. Kiedrowski
14:40-15:05	P. Griffin
15:05-15:30	M.E. Rising
15:30-16:00	Coffee Break
Section	Astrophysics
Chair	T. Kawano
16:00-16:30	N. Schunck
16:30-16:55	B. Pritychenko
16:55-17:25	M.R. Mumpower

Wednesday, April 30, 2014

Section Chair	Advanced Fission Experiments at LANSCE M.C. White
9:00-9:30 9:30-9:55 9:55-10:20	F. Tovesson R.C. Haight T.N. Taddeucci
10:20-10:50	Coffee Break
Section Chair	Experimental Covariance Estimation & Nuclear Data Evaluations R. Capote
10:50-11:20 11:20-11:45 11:45-12:10 12:10-12:35	T. Burr D. Neudecker Y. Zhang H. Leeb
12:35-14:05	Lunch Break
Section Chair	Nuclear Data Evaluations Including Covariances A.D. Carlson
14:05-14:35 14:35-15:00 15:00-15:25	S. Kunieda G.M. Hale A. Sonzogni
15:25-15:55	Coffee Break
Section Chair	Nuclear Data Evaluation Methodology G.M. Hale
15:55-16:25 16:25-16:55 16:55-17:20	P. Schillebeeckx C. De Saint Jean G. Žerovnik
17:20-19:00	Break
19:00-22:00	Conference Dinner

Thursday, May 1, 2014

Section Chair	Nuclear Data Evaluation Methodology D. Neudecker
9:00-9:30 9:30-9:55 9:55-10:20	D. Higdon S. Varet G. Schnabel
10:20-10:50	Coffee Break
Section Chair	Nuclear Data Evaluation Methodology D.L. Smith
10:50-11:20 11:20-11:50 11:50-12:15	E. Bauge A. Koning P. Helgesson
12:15-13:45	Lunch Break
Section Chair	Evaluations of Fission Product Yields P. Talou
13:45-14:15 14:15-14:40 14:40-15:05	S. Pomp N. Terranova M.T. Pigni
after 15:05	Farewell

Application of the COMMARA-2.1 Data to Uncertainty Evaluation of Fast System Integral Parameters

G. Aliberti

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A set of cross section covariance data is being developed in a 33-group structure at BNL and LANL. The present work aims to show the application results of the latest release of the covariance data, called COMMARA-2.1 [1], to the uncertainty evaluation of the main integral parameters of a series of fast systems investigated in recent sensitivity studies [2, 3]. For a 1000 MWt Advanced Burner Reactor (ABR) loaded both with metal and oxide fuel, a 840 MWt sodium cooled reactor (SFR) with low transuranic (TRU) conversion ratio, a 3600 MWt sodium cooled European Fast Reactor (EFR), a 2400 MWt gas cooled fast reactor (GFR), a 900 MWt lead cooled fast reactor (LFR) and a 377 MWt accelerator-driven minor actinide burner (ADMAB), the uncertainties of multiplication factor, power peak, Doppler reactivity worth, coolant void reactivity worth, burnup reactivity worth, decay heat at 100 years after discharge, neutron source at 2 years after discharge and neutron dose at 100000 years after discharge will be evaluated with the COMMARA-2.1 covariance data and compared with those obtained with the previous version of the matrix, COMMARA-2.0 [4]. Sensitivity coefficients for most of the considered integral parameters were already obtained in the Subgroup 26 studies using the JEF3.0 and JEF2.0 data libraries for the cross section processing [2]. Sensitivities of all integral parameters have been re-evaluated in the present analysis with a consistent use of the ENDF/B-VII.0 nuclear data [5]. Sensitivities are determined with respect to ν, fission, capture, elastic and inelastic scattering, n,2n and χ. To identify the most important reactions to the uncertainty of the investigated integral parameters, the contributions of individual reaction types is being investigated. From the analysis of the multiplication factors it is found that the overall uncertainties estimated with COMMARA-2.1 show negligible discrepancies with respect to the COMMARA-2.0 results, except in the case of the SFR and ADMAB reactors. Using the COMMARA-2.0 covariance matrix, the overall multiplication factor uncertainty increases from 0.78% to 1.13% in the case of SFR, and from 1.19% to 1.78% in the case of ADMAB. The observed discrepancy is quite relevant, since it implies a difference of about 500 pcm in the estimated uncertainties on the multiplication factors of these two reactors. From the breakdown by isotope and reaction of the SFR multiplication factor it appears that using the COMMARA-2.0 data the change in the obtained uncertainties is particularly due to ^{245}Cm fission (increase in the uncertainty contribution from 0.05% to 0.49%), to ^{240}Pu ν (increase from 0.13% to 0.47%) and fission (increase from 0.10% to 0.27%), ^{238}Pu ν (increase from 0.06% to 0.17%) and ^{23}Na capture (decrease from 0.10% to 0.00%). Similarly, concerning the discrepancies

in the estimated uncertainties with the COMMARA-2.0 compared to the COMMARA-2.1 covariance matrix in the case of the ADMAB multiplication factor, the most relevant effects are associated with ^{245}Cm fission (increase in the uncertainty contribution from 0.11% to 1.08%), to ^{244}Cm fission (increase from 0.15% to 0.66%) and capture (increase from 0.32% to 0.52%) and ^{237}Np capture (decrease from 0.32% to 0.19%). In the full paper the uncertainty analysis will be extended to the other integral parameters as well. For a better understanding of the observed discrepancies between the uncertainties estimated with two sets of covariance data, relative standard deviations of the most relevant reactions will be also compared. For the reactions of most interest, the energy distributions of the obtained uncertainty will be investigated. Finally, based on the application results of COMMARA-2.1, suggestions will be eventually addressed to the evaluators for further improvements of the covariance data.

References

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Covariance Matrix of Thermal Neutron Scattering Kernel

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We will present methods for generating covariance matrices of thermal neutron scattering kernels for materials of interest in nuclear applications. We will compare covariance matrices obtained using these methods, including molecular dynamics simulations, and the density functional theory. We will report on work in progress related to evaluation of covariance matrix based on the data being measured at the ORNL Spallation Neutron Source.

"Full model" nuclear data and covariance evaluation process, using TALYS, Total Monte-Carlo and Backward-Forward Monte-Carlo.

E. Bauge

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The "Full model" evaluation process [1], that is used in CEA DAM DIF to evaluate nuclear data in the continuum region, makes extended use of nuclear models implemented in the TALYS [2] code to account for experimental data (both differential and integral) by varying the parameters of these models until a satisfactory description of these experimental data is reached. For the evaluation of the covariance data associated with this evaluated data, the Backward-Forward Monte-Carlo (BFMC) method [3] was devised in such a way that it mirrors the process of the "Full model" evaluation method. When coupled with the Total Monte-Carlo [4] method via the T6 [5] system, the BFMC method allows to make use of integral experiments to constrain the distribution of model parameters, and hence the distribution of derived observables and their covariance matrix. Together, TALYS, TMC, BFMC, and T6, constitute a powerful integrated tool for nuclear data evaluation, that allows for evaluation of nuclear data and the associated covariance matrix, all at once, making good use of all the available experimental information to drive the distribution of the model parameters and the derived observables.

References

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Exploring the role of nuclear data uncertainties in ultra-high resolution gamma spectroscopy for isotopic analysis using approximate Bayesian computation

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High Purity Germanium currently provides the highest readily available resolution gamma detection for a broad range of radiation measurements, but microcalorimetry is a developing option that has considerably higher resolution. Superior resolution offers the potential to better distinguish closely spaced x-rays and gamma-rays, a common challenge for the low energy spectral region from special nuclear materials, and the higher signal-to-background ratio confers an advantage in detection limit. As microcalorimetry continues to develop, it is timely therefore, to reassess the role of uncertainties in detector/item response functions and in basic nuclear data, such as branching ratios and half-lives, used to interpret spectra in terms of the contributory radioactive isotopes. We illustrate that a new inference option known as approximate Bayesian computation (ABC) is effective and convenient both for isotopic inference and for uncertainty quantification for microcalorimetry. The ABC approach opens a pathway to new and more powerful implementations for practical applications than currently available.

Current issues on nuclear data evaluation methodology and applications to cross section and PFNS evaluations

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Modern evaluations of nuclear data need to combine knowledge embedded in both the experimental data and/or nuclear models. A methodology to evaluate nuclear data producing the average values and corresponding uncertainty and covariance data of relevant physical quantities is reviewed. Outstanding issues are discussed including model uncertainties (beyond model parameter uncertainties), treatment of cross section fluctuations, experimental covariance assessment, and evaluation of normalized quantities (e.g. PFNS). Applications of the evaluation methodology are shown for neutron induced reactions on manganese, and for PFNS evaluation of ^{233,235}U and ^{239}Pu thermal-neutron induced fission. Impact of new evaluations on on-going CIELO project is discussed.

Recent Work Leading Towards a New Evaluation of the Neutron Standards

A.D. Carlson[1], V.G. Pronyaev[2], R. Capote[3], G.M. Hale[4], F.-J. Hambsch[5], T. Kawano[4], S. Kunieda[6], W. Mannhart[7], R.O. Nelson[8], D. Neudecker[4], P. Schillebeeckx[5], S. Simakov[3], D.L. Smith[9], P. Talou[4], X. Tao[10], A. Wallner[11,12], W. Wang[10]

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A new version of the ENDF/B library has been planned. The first step in producing this new library is evaluating the neutron standards. A new international evaluation of the neutron standards is now underway with support from a Data Development Project of the IAEA. In addition to the neutron cross section standards, new evaluations are being done for the ^{252}Cf spontaneous neutron spectrum standard. Also work is being done on a number of reference data. These data are not known as well as the standards but are often used in ratio measurements instead of the standards since they are somewhat more convenient to use. They include an extension of the energy range of the gold capture cross section, reference cross sections for use in gamma ray production cross section measurements (e.g. inelastic scattering cross sections), and the ^{235}U thermal neutron induced neutron spectrum.Efforts have been made to handle uncertainties in a proper way for these evaluations. For example, for the comprehensive evaluation of the neutron cross section standards, correlations are taken into account as a function of energy for each cross

section and for known correlations with other cross sections. The data in the evaluation also include the ^{238}U(n,γ) and ^{239}Pu(n,f) cross sections in addition to the standard cross sections. Those data were included since there are many ratio measurements of those cross sections with the standards and absolute data are available on them. The work done in this project will be discussed.

Variance reduction factor of nuclear data for integral neutronics parameters

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In the present paper, we propose a methodology to identify which nuclear data should be further improved to reduce the variance of the target integral neutronics parameters. Using covariance matrix of nuclear data and the conventional cross section adjustment theory we can quantify how much new microscopic nuclear data measurement contributes to the reduction of the variance of target integral neutronics parameters. This method cannot quantify the target accuracy for the microscopic nuclear data like the inverse sensitivity/uncertainty computation methodology, but this method takes into account the correlation between the nuclear data, which is ignored in the inverse method.

Physical Constraint on Covariance's evaluation : from microscopic to integral experiments

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In neutron induced reactions between 0 eV and 20 MeV, a general problem arises during the evaluation of cross sections. The evaluation work may be done independently between the resolved resonance range and the continuum, giving rise to mismatches for the cross sections, larger uncertainties on boundary and no cross-correlations between high energy domain and resonance range. This paper will present several methodologies that could be used to avoid such effects. A first idea based on the use of experiments systematic uncertainties(normalization for example) overlapping two energy domains will be presented. Then a methodology based on Lagrange multipliers is proposed to take into account physical constraints on an overlapping energy domain where two nuclear reaction models are used (continuity of both cross sections or derivatives for example). A last, a review of the use of integral experiments as physical additional constraints during the evaluation of covariances will be presented as well as the related issues.

Nuclear Data Uncertainty Propagation in Transmutation Calculations of Advanced Reactor Systems with Comparison of using One-Group or Multi-Group Cross Sections

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Several approaches have been developed in the last several years in order to tackle the nuclear data uncertainty propagation problems of burnup calculations. One approach proposed was an hybrid method, where the uncertainties on nuclear data are only propagated through the depletion part of a burnup problem (which coupled transport and depletion problem). Due to the fact that only the depletion part is overcome, only one-group cross sections are required for such part, and therefore, their collapsed one-group uncertainty. This approach has been applied successfully in several advanced reactor systems like EFIT (ADS-like reactor) or ESFR (Sodium fast reactor) to assess the uncertainty on the isotopic composition due to nuclear data. However, the comparison with the uncertainty propagation using the multi-group structure was not performed, and then, it is going to be presented here in this work for the ESFR case. Furthermore, the improvement in the hybrid method done for tackling problems with burnup problems with neutron spectrum variations using one-group cross sections is assessed when large variations of the spectrum take place, and it is compared against when multi-group cross sections are used instead.

Integral Benchmark Experiments in the Inverse Sensitivity/Uncertainty Computations

M.E. Dunn[1], G. Arbanas[1], B.A. Khuwaileh[2], M.L. Williams[1], L.C. Leal[1], C. Wang[2], H.S. Abdel-khalik[2]

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The inverse sensitivity/uncertainty quantification (IS/UQ) method aims to find the required uncertainties of the cross section data that are to yield a target uncertainty of a nuclear applications response, at a minimum cost of acquiring the required data uncertainties. However, in some cases the extant uncertainties of the cross section data are already near the limits of the present-day state-of-the-art measurements, and requiring the uncertainties to be significantly smaller may be unrealistic. In order to avoid this scenario, we have incorporated integral benchmark experiment (IBE) data into the IS/UQ method using the generalized linear least-squares method. We show that inclusion of the IBE into IS/UQ method yields less stringent uncertainties while still achieving the applications target accuracy. We compute the effect of IBEs on the IS/UQ applied to a thermal nuclear system (i.e., pressurized water reactor (PWR) fuel type). However, this method can be applied to other nuclear systems or more generally.

Progress, challenges, excitement and perspectives in developing nuclear data covariances in the Indian context

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The topic of covariances is new to Indian nuclear and reactor physics communities. Currently unique efforts are being made in India in bringing together scientists in various fields such as in nuclear physics experiments, nuclear theory and statistical inferences to learn together the basics of nuclear data covariances and to evolve a sound and sustainable program. This presentation attempts to cover the progress, challenges, excitement and perspectives in understanding and developing nuclear data covariances in the Indian context. The talk will also present the authors perspectives on the role and importance of nuclear data covariances in the Indian context in advanced reactor design physics applications. The talk will also mention experiences in the recently published international criticality benchmarking of Indian reactors. The indigenous efforts in India on covariances cover and influence broadly the following topics:

- Nuclear data physics experiments including surrogate reactions; Cross section measurements, covariances.
- Measured raw data compilations in EXFOR format; Covariances.
- Cross-section evaluations include use of nuclear models, statistical inference tools, and covariances based on nuclear models.
- Understanding formats and procedures; Processing of covariances
- Neutron-photon coupled transport calculations and response functions. Reactor Design with the use of plug-in covariance nuclear libraries. Reactor sensitivity studies.
- Use of covariances to define error margins due to uncertainties in nuclear data and adjustment of cross-sections. Perspectives on uncertainties in quantities other than nuclear data, affecting target accuracies in advanced reactor designs.
- Creation of Indian experimental benchmarks with specification of uncertainties in system characterization. Integral experiments with covariances.

The subject of nuclear data covariances is recognized as an important part of several ongoing nuclear data science activities in Nuclear Data Physics Centre of India (NDPCI) since 2007. A Phase-1 project in collaboration with the Statistics department in Manipal University, Karnataka (Prof. K.M. Prasad and Prof. S. Nair) on nuclear data covariances was executed successfully during 2007-2010 period. In Phase-1, the emphasis was on a thorough basic understanding of the concept of covariances including assigning uncertainties to experimental data in terms of partial errors and micro correlations, thorough a study and a detailed discussion of open literature. Towards the end of Phase-1, measurements and a first time covariance analysis of cross-sections for ^{58}Ni(n,p)^{58}Co reaction measured in Mumbai Pelletron accelerator using ^{7}Li(p,n) reactions as neutron source in the MeV energy region were performed under a PhD program on nuclear data covariances in which enrolled are two students, Shri. B. S. Shivashankar and Ms. Shanti Sheela. India is also successfully evolving a team of young researchers to code nuclear data of uncertainties, with the perspectives on covariances, in the IAEA-EXFOR format. The NDPCI has conducted three national Theme meetings sponsored by the DAE-BRNS in 2008, 2010 and 2013 on nuclear data covariance. A Phase-II DAE-BRNS-NDPCI proposal of project at Manipal is being evolved at this time. In Phase-2, modern nuclear data evaluation techniques will be further studied as a research and development effort, as a first time effort. The talk summarizes the progress achieved thus far in the learning curve of these exciting efforts.

Covariance Propagation in Spectral Indices

P. Griffin

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In reactor neutron reference benchmark fields [1], spectrum-averaged cross sections for reactions of interest to the dosimetry community are often given in the form of a spectral index (SI), that is, as a ratio of the spectrum-averaged cross section for the given detection reaction to that for a reference reaction [2]. This quantity is often used because it removes the sensitivity of the metric to the reactor power or to any dependence on an absolute fluence diagnostic. This provides an experimental metric that is sensitive to the spectral shape and has a low measurement uncertainty. However, the calculated-to-experimental (C/E) double ratio is often the quantity required to validate either a neutron spectrum or a cross section determination. In calculating the uncertainty in this double ratio, the uncertainty in the calculated spectral index typically neglects to consider the uncertainty due to the knowledge of the neutron spectrum. Arguments can be made that this uncertainty cancels out when the sensitivity of the test cross section is similar to that for the reference reaction. However, this condition of similar sensitivity can be very dependent upon the spectral shape. The definition of a spectral definition in Reference 1 states that it is applicable among detector pairs with distinguishable energy response ranges, and this is clearly in conflict with the similarity condition and supports the observation that this similarity is violated in the majority of cases where SIs are reported for reactor-based reference neutron fields. This paper examines the importance of the spectrum uncertainty in reporting uncertainties in the C/E ratios for SIs for reactions of interest to the dosimetry community. When proper a priori information is available for the reference neutron field, i.e. a covariance matrix, we show how one can rigorously treat the uncertainty propagation in this double ratio. Data is reported for two reference neutron fields for Sandia reactors, the Sandia Pulsed Reactor (SPR-III) central cavity, a fast burst reactor assembly, and the Annular Core Research Reactor (ACRR), a water moderated pool-type reactor with a large dry central cavity [3].

References

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The Chi-Nu Program to Measure Prompt Fission Neutron Spectra and Provide Detailed Associated Uncertainties – Progress and Plans[1]

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New data on the prompt fission neutron spectra (PFNS) from neutron-induced fission with higher accuracies are needed to resolve discrepancies in the literature and to address gaps in the experimental data. The Chi-Nu project, conducted jointly by LANL and LLNL, aims to measure the shape of the PFNS for fission of ^{239}Pu induced by neutrons from 0.5 to 20 MeV with accuracies of 3-5% in the outgoing energy from 0.1 to 9 MeV and 15% from 9 to 12 MeV and to provide detailed experimental uncertainties. Neutrons from the WNR/LANSCE neutron source are being used to induce fission in a Parallel-Plate Avalanche Counter (PPAC). Two arrays of neutron detectors are used to cover the energy range of neutrons emitted promptly in the fission process. Challenges for the present experiment include background reduction, use of ^{239}Pu in a PPAC, and understanding neutron detector response. Achieving the target accuracies requires the understanding of many systematic uncertainties. The status and plans for the future will be presented.

[1]This work is performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and the Los Alamos National Laboratory under Contract DE-AC52-06NA25396.

Data Covariances from R-Matrix Analyses of Light Systems

G.M. Hale, M.W. Paris

T-Division, Los Alamos National Laboratory, Los Alamos, NM, USA

We will first review the parametric description of light-element reactions in multichannel systems using R-matrix theory. The general LANL R-matrix analysis code EDA provides accurate covariance information for the resonance parameters at a solution due to the rank-one variable-metric search algorithm it uses to find a local minimum of the chi-square surface. This information is used, together with analytically calculated sensitivity derivatives, in the first-order error propagation equation to obtain cross-section covariances for all reactions included in the analysis. Examples will be given of the covariances obtained for systems with few resonances (^{5}He) and with many resonances (^{13}C or ^{17}O). We will discuss the prevalent problem of this method leading to cross-section uncertainty estimates that appear to be unreasonably small for large data sets.

Properly including experimental uncertainties in the TMC methodology

P. Helgesson
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Total Monte Carlo (TMC) [1] is a method for propagating nuclear data uncertainties based on sampling of nuclear model parameters. It is easy to implement using the publicly available random files from the TENDL project [2] and it has been applied to a wide range of applications. However, since the introduction of the method, some criticism has been directed towards it because experimental data have not been taken into account in a statistically well-founded manner, see e.g. Ref. [3]. This work addresses this critique by suggesting how to properly include both differential and integral experimental data and its uncertainties in the TMC methodology. The foundation of the method, similar to that in e.g. Unified Monte Carlo (UMC)[4], is to modify a prior distribution for the nuclear model parameters using Bayes' theorem. This is in principle simple, but several practical concerns arise, most of which are discussed in this work. The likelihood function to use in Bayes' theorem is derived from the assumption that the full set of experiments can be described by a multivariate Gaussian. Unfortunately, very few EXFOR [5] entries are provided with estimates of experimental correlation matrices and cross-experimental correlations are even harder to obtain. However, information distinguishing between statistical and systematic uncertainty is often available as well as information on monitor cross sections. A set of simple and mildly conservative rules is suggested to determine which experimental correlations to use, given the limited information. Further, a way to include the correlative effect of monitor cross sections is suggested as it is an important contribution to the cross-experimental correlation of errors. Since sampling from a general high-dimensional distribution is computationally heavy, it is proposed to sample *implicitly* from the posterior distribution by assigning weights to the TENDL random files and to use a Russian Roulette procedure to avoid computations with an impractically low weight. This is shown to asymptotically give the correct result and the uncertainty of the uncertainty can be quantified to handle the finite number of realizations. The choice of prior distribution is discussed, and a general criterion for a "too narrow" prior is suggested to ensure that no unjustified constraints are assigned to the nuclear data. Further, a method to sample systematic uncertainties to avoid problematic matrix inversions is presented and

this is compared to the more conventional approach. The method, with some temporary simplifications, is implemented and used to propagate uncertainties in a simple PWR pin cell model.

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Covariances in ENDF/B-VII.1: status, concerns and future

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The status of covariances in the ENDF/B-VII.1 library will be reviewed in regard to the methods used to determine the uncertainties and their correlations. Actinides, fission products and structural materials will be discussed with an emphasis on uncertainty quantification in the fast neutron range. Recent developments that lead to the set of covariances in ENDF/B-VII.1 will be outlined. In particular, I will address the diversity of methods used in these covariances, which improved considerably without a well-established methodology. These efforts were often the result of contradictory aspects of the current situation, such as a demand for covariances in support of applications in spite of limited resources, a need for complete covariances, including cross-reaction and cross-material correlations, and the proper inclusion of experimental covariances (and the practical difficulty of determining them for old measurements), all of which face the technical difficulties associated with the handling such large entities. I will try to summarize major shortcomings of the current covariance landscape showing that while we have achieved substantial improvement over recent years we are still far from the ultimate goal.

A Statistical Perspective in Assessing Uncertainties in Physical Constants

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This talk will give a general overview of statistical approaches for assessing uncertainties in model parameters. Both classical and Bayesian approaches will be considered, along with the computational recipes used by these approaches. Time permitting, I'll give examples from physics-based applications.

Integral Data Assimilation and Covariances

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A study is underway at the NNDC at Brookhaven National Lab to investigate the use of both differential and integral experimental data to produce 'unified' reaction cross sections that will reproduce both types of experimental observables without further need for adjustment. The method fits the data by first determining the sensitivity of the observables to the varied EMPIRE model parameters and then fitting these parameters to the experimental data using Kalman updates. For integral data this involves propagating the EMPIRE results to Monte-Carlo simulations of integral experiments, so as to determine the sensitivity of integral observables to the model parameters directly. Obtaining good agreement with integral data often requires fitting many integral observables simultaneously while varying multiple materials. The resulting covariance matrix of fitted parameters can then be used to calculate not only covariances for the modeled reactions, but also cross-reaction and cross-material covariances for any reaction and material that were varied in the fit. We will present initial results of these multiple material, multiple experiment fits and the resulting covariances.

Efficient Subspace based Algorithm for Targeted Accuracy Nuclear Data Assessment using Inverse Uncertainty Quantification

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Safety analysis and design optimization depend on the accurate prediction of various reactor attributes. Predictions can be enhanced by reducing the uncertainty associated with the attributes of interest. An inverse problem can be defined and solved to assess the sources of uncertainty; and experimental effort can be subsequently directed to further improve the uncertainty associated with these sources. In this work a subspace-based algorithm for inverse sensitivity/uncertainty quantification (IS/UQ) has been developed to enable analysts account for all sources of nuclear data uncertainties in support of target accuracy assessment-type analysis. An approximate analytical solution of the optimization problem is used to guide the search for the dominant uncertainty subspace. By limiting the search to a subspace, the degrees of freedom available to the optimization search are significantly reduced. The proposed algorithm is compared with a conventional IS/UQ algorithm to search the full uncertainty space. A quarter PWR fuel assembly is modeled and the accuracy of the multiplication factor and the fission reaction rate are used as reactor attributes whose uncertainties are to be reduced. Numerical experiments are used to demonstrate the computational efficiency of the proposed algorithm. Our ongoing work is focusing on extending the proposed algorithm to account for various forms of feedback, e.g., thermal-hydraulics and depletion effects.

Critical Experiment Sensitivity/Uncertainty Analysis with Continuous-Energy Monte Carlo

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Critical experiments in conjunction with continuous-energy Monte Carlo methods are one of the means by which the quality of neutron nuclear data can be assessed. Recent developments have led to the ability to provide first-order perturbation estimates of prior calculation uncertainties resulting from the nuclear data covariances of the effective multiplication k_{eff}. Optimization techniques can be applied considering both the experimental and data uncertainties and correlations to provide proposed nuclear data libraries that best match experimental data. This proposed library can be used by evaluators to guide their expert judgment for creating their data libraries. Additionally, statistical tests can be used to help validate the covariance data itself as well; large disagreement with experiment relative to the nuclear data uncertainty may indicate problems with the covariance data.

New developments in Monte Carlo uncertainty propagation

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Various methods for uncertainty generation with Monte Carlo methods are compared on a consistent basis: These include the already existing Unified Monte Carlo, and Backward-Forward Monte Carlo methods, but also new techniques will be discussed. One of the novelties is that sampling is done from arbitrary parameter distributions, which are formed through a self-learning mechanism using EXFOR-based weights. As usual, the method has been applied to all nuclides at once, thereby improving the next TENDL nuclear data library.

Once the scheme for uncertainties for differential data, coming from both models and experiments, is established, we will demonstrate the latest possibilities of Total Monte Carlo: the original application to criticality benchmarks is now extended among others to reactor burnup profiles and nuclear accident related scenarios. Finally, we will show how Total Monte Carlo provides a natural way to reduce integral uncertainties for a specific reactor, or other, case by using integral benchmarks, and how evaluations can be optimized using Monte Carlo, using ^{239}Pu as an example.

Covariance of Neutron Cross-section for ^{16}O through R-matrix Analysis

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The collision matrix in the R-matrix theory is unitary, hence theory brings strong constraints to behavior of the parameters. An unitarity-imposed R-matrix analysis is carried out for ^{17}O system to evaluate ^{16}O neutron cross-sections in the resolved resonance range. Covariance matrices are also estimated both for the cross-sections and angular distributions with a deterministic method. Present results mirror the nature in the theory as well as experimental information.

Bayesian evaluation including covariance matrices of neutron-induced reaction cross sections of ^{181}Ta[2]

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A new evaluation of neutron-induced reactions on ^{181}Ta using a consistent procedure based on Bayesian statistics is presented. Starting point of the evaluation is the description of nuclear reactions via nuclear models implemented in TALYS. Especially, a coupled-channel formalism is applied for the ground state and the lowest collective states. An optical model of the form of Koning and Delaroche with slightly adjusted parameters is used together with the CTM level densities. An extensive retrieval of experimental data was performed and covariance matrices of the experiments were generated from an extensive study of the associated literature. All relevant reaction channels and spectra up to 200 MeV have been considered and the corresponding covariance matrices determined. A comparison with experimental data and available evaluations is given together with the associated covariance matrices. While the correlations essentially reflect the mutual relationships, it must be remarked that in general variances, especially in less well described reaction channels, are similarly to other evaluation techniques too small. An improved formulation of model defects which conserves sum rules is required to account for this deficiency. Using the results of the evaluation a complete ENDF-file similarly to those of the TENDL library is generated.

[2]The work has been supported by Fusion for Energy Partnership Agreement via the grant F4E-FPA-168.01. The views and opinions herein do not necessarily reflect those of the European Commission.

Handling covariances in Fudge and GND

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The Generalized Nuclear Data infrastructure (GND) is being designed as a new standard for storing nuclear data. It is intended as an eventual replacement for the ENDF-6 standard, and must be capable of handling all types of data supported by ENDF-6. Formats for storing covariances in GND are currently under active development. The final format must be concise yet easy to read and use. We will present on the status of covariances in GND, and on the tools for generating and using covariance data that are being implemented in LLNL's nuclear data toolkit 'Fudge'.

The sensitivity of a main r-process to nuclear masses near closed shells[3]

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Nuclear masses are one of the key ingredients of nuclear physics that go into astrophysical simulations of the r-process. Nuclear masses effect r-process abundances by influencing Q-values, neutron capture rates, photo-dissociation rates, beta-decay rates and the probability to emit neutrons. Most of the thousands of short-lived neutron-rich nuclei which are believed to participate in the r process lack any experimental verification, thus the identification of the most influential nuclei is of paramount importance. We have conducted mass sensitivity studies near closed shells in the context of a main r-process component which could occur in supernova or compact object mergers. Our studies take into account how an uncertainty in a single nuclear mass propagates to influence the relevant quantities of neighboring nuclei and finally to r-process abundances. Using various nuclear models and astrophysical conditions we identify key nuclei in these studies whose mass has a substantial impact on final r-process abundances and discuss implications for measurements at radioactive beam facilities.

[3]This work was supported by the Joint Institute for Nuclear Astrophysics grant number PHY0822648.

Evaluation and Uncertainty Quantification of the Prompt Fission Neutron Spectrum of ^{239}Pu for incident neutron energies up to 30 MeV

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For the ENDF/B-VII.1 library [1], significant efforts were undertaken to provide evaluated covariances for many reactions and isotopes, including the prompt fission neutron spectrum (PFNS) of ^{239}Pu induced by neutrons of 0.5 MeV [2]. The evaluated covariances were obtained by combining Los Alamos model (LAM) calculations [3] and experimental knowledge, albeit both model and experimental covariances were estimated based on some simplifying assumptions.

Here we present preliminary results of a ^{239}Pu PFNS evaluation where special emphasis was placed on a thorough uncertainty quantification. Experimental covariance matrices were estimated carefully using available literature as well as in close collaboration with experimentalists. Uncertainties of additional model parameters were considered for the model covariances. In addition, the LAM was extended to include an anisotropy in the emission of the neutrons in the center of mass of the fragment, as well as different temperature distributions in the light and heavy fragments [4]. The incident energy dependence of LAM input parameters was studied to provide consistent model data for several incident energies up to 30 MeV. The evaluated mean values, covariances and mean energies are compared to existing data files and experimental information. The evaluated results at thermal incident neutron energy are also compared to a statistical analysis using primarily experimental data to study the impact of model information on the evaluated mean values and covariances.

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A-priori and a-posteriori covariance data in nuclear cross section adjustments: issues and challenges

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The role for cross section adjustment is more and more perceived as that of providing useful feedback to evaluators and differential measurement experimentalists in order to improve the knowledge of neutron cross sections to be used in a wider range of applications. This new role for cross section adjustment requires tackling and solving a new series of issues: definition of criteria to assess the reliability and robustness of an adjustment; requisites to assure the quantitative validity of the covariance data; criteria to alert for inconsistency between differential and integral data; definition of consistent approaches to use both adjusted data and a-posteriori covariance data to improve quantitatively nuclear data files; provide methods and define conditions to generalize the results of an adjustment in order to evaluate the extrapolability of the results of an adjustment to a different range of applications (e.g., different reactor systems) for which the adjustment was not initially intended; suggest guidelines to enlarge the experimental data base in order to meet needs that were identified by the cross section adjustment. In order to satisfy these requirements, several methodology issues will be illustrated with practical examples. Among them:

- Assessment of adjustments by the means of several useful parameters (e.g., adjustment margin, individual χ^2, experiment contribution to a priori and a posteriori χ^2, etc.)
- Definition of criteria to accept new central values of cross sections after adjustments (e.g., consistency with other evaluated data files and differential measurements, variation to be consistent with the initial standard deviation, etc.)
- Avoid compensation among different nuclear data adjustments (e. g. make sure that all reactions and physical phenomena are taken into account, use a comprehensive and representative set of experiments, etc.)

- Validation of the a priori covariance matrix (e.g., by χ^2 of the adjustment, and consistency between cross section variation and standard deviation) and use of the a posteriori covariance matrix. Assess the new covariance matrix physical meaning. Use of the new correlations between cross sections and experiments obtained after the adjustment.

- Issues related to the presence of negative eigenvalues in the a priori covariance matrix.

^{235}U Fission Product Yield Covariance Data for the Thermal Neutron Range[4]

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Reliable fission product yields (FPYs) are important to understand and predict the fission process in a nucleus at intermediate energies for nuclear energy applications. Increasing demands for reliable FPY data come primarily from nuclear energy safety applications [1][2] as well as radiological source terms relevant to nuclear security, nuclear forensic analysis, non-proliferation research, and recent and growing interest in transportation, storage, and geologic disposal of radioactive waste. Research on fission product yield *uncertainties* and related *correlations* is also an emerging area of high interest to international organizations engaged in used fuel analysis. Organization for Economic Co-operation and Development has recently initiated a new subgroup under the Working Party on International Nuclear Data Evaluation Co-operation on fission product yield uncertainties, namely WPEC-37. Oak Ridge National Laboratory is currently working on developing methodologies to generate covariance matrices on FPY data [3], in collaboration and with guidance from several organizations involved in similar efforts, including the University of Madrid [4], United Kingdom National Nuclear Laboratory [5], Los Alamos National Laboratory [6], and Schmidt [7]. The Japan Atomic Energy Agency has also been involved in fission yield uncertainty analysis through the work of Katakura [2]. In view of its importance in reactor safety and used fuel studies, ^{235}U was selected as the test material to estimate independent fission product yield covariance matrix in the thermal neutron range. Our evaluation used the combination of the five Gaussian and Whal model [8] to describe the mass and charge distribution of the FPY data. The parameters of this semi-empirical model were primarily used to define an estimate of covariance matrix for independent FPY data for which the ENDF/ B-VII.1 evaluation serves as the reference. Independent FPY data are usually associated with uncertainties larger than cumulative FPY data. In order

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to account for the decay processes that result in the cumulative FPY data of the lower-uncertainty long-lived fission products, we updated the covariance matrix for independent FPY through a non-iterative retroactive Bayesian method. Both uncertainties and related correlations obtained with this method provide internal consistency between independent FPY uncertainty data and cumulative FPY ones.

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Studies of the impact of fission yield uncertainties on the nuclear fuel cycle with TALYS/GEF and the TMC method

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The TMC methodology allows propagation of uncertainties from the microscopic to the macroscopic world. Using TALYS which, in the latest release, partially includes the GEF code, it is possible to assess the impact of the limits of our knowledge of fission yields on, e.g., the nuclear fuel cycle. Besides state-of-the-art nuclear model codes, high-quality experimental data are needed for model guidance, to constrain parameter space, and to reveal dependences of physics parameters on energy and fission system. In addition, TMC with experimental data as benchmark can also be used to study parameter correlations.

The nuclear reactions research group at Uppsala University is involved in experimental activities measuring fission yields in the fast energy range from ^{232}Th, ^{234}U, and ^{238}U with Frisch-grid ionization chambers. Currently we work on developing methods to measure independent fission yields in a fast-reactor-like neutron spectrum at the IGISOL facility in Jyväskylä, Finland.

In this paper we describe our research program concerning nuclear model uncertainties for fission yields and their impact on the fuel cycle and present first results of using GEF with the TMC method for analysis of our experimental data. We will also give an overview of planned measurements at IGISOL.

Calculations of Nuclear Energy and Astrophysics Neutron Cross Section Uncertainties using ENDF/B-VII.1 and Low-Fidelity Covariances

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^{252}Cf and nuclear astrophysics neutron cross sections and their uncertainties have been calculated for several nuclear data applications. Absolute values were deduced with Mannhart and Maxwellian formalisms, while uncertainties are based on ENDF/B-VII.1 and Low-Fidelity covariances. These quantities are compared with nuclear data standards, independent benchmarks, EXFOR library, and analyzed for a wide range of cases. Recommendations for neutron cross section covariances will be given and implications will be discussed.

A Comparison of Sensitivity Analysis and Uncertainty Propagation Methods with respect to the Prompt Fission Neutron Spectrum Impact on Critical Assemblies

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While many of the modern nuclear data libraries, such as the ENDF/B-VII.1 library in the US [1], now include covariance data [2], there remains a need to study the various ways to use the information given in the evaluated covariances. Calculating the total uncertainties of an integral quantity dependent on the nuclear data of interest is one common use of covariance data. Another possible use of the available covariance data is to compute the cross-covariance between the inputs (nuclear data) and outputs (integral quantities), which would offer higher-order uncertainty information. This kind of information could be used to provide feedback to experimentalists and theorists on where the improvements can be made to the nuclear data. Compared to standard sensitivity analysis, where the sensitivity profile of the integral responses are generally based on uncorrelated perturbations of nuclear data, this method is informed by the evaluated covariance matrix and could provide a more appropriate feedback mechanism.

In the present work, the prompt fission neutron spectrum (PFNS) uncertainties in the n+^{239}Pu fission reaction are used to study the impact on the Jezebel fast critical sphere assembly modeled in the MCNP6 [3] code. The newly developed sensitivity capability [4] is used to compute the k-eigenvalue sensitivity coefficients with respect to the PFNS. In comparison, the covariance matrix given in the ENDF/B-VII.1 library is decomposed and randomly sampled realizations of the PFNS are propagated through the criticality calculation, preserving the PFNS covariance matrix. The information gathered from both methods, including the overall k-eigenvalue uncertainty, is statistically analyzed. Numerical results are presented along with a discussion regarding the similarities and differences in the sensitivity analysis and uncertainty propagation techniques. Feedback is provided regarding the regions for which the PFNS would have the largest impact on the particular integral quantities studied in the present work.

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The role of uncertainty quantification for reactor physics

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The role of uncertainty quantification has been stressed and has been the object of several assessments in the past (see e.g. Reference [1] and [2]), in particular in relation to design requirements for safety assessments, design margins definition and optimization, both for the reactor core and for the associated fuel cycles. The use of integral experiments has been advocated since many years, and recently re-assessed (Ref. [3]) in order to reduce uncertainties and to define new reduced a-posteriori uncertainties. While uncertainty quantification in the case of existing power plants benefits from a large data base of operating reactor experimental results, innovative reactor systems (reactor and associated fuel cycles) should rely on limited power reactor experiment data bases and on a number of past integral experiments that should be shown to be representative enough. Moreover, in some cases, in particular related to innovative fuel cycle performance and feasibility assessment, nuclear data uncertainties are the only available information. Uncertainty quantification in that case becomes a tool for detecting potential show stoppers associated to specific fuel cycle strategies, besides the challenges related to fuel properties, fuel processing chemistry and material performance issues. As an example of uncertainty quantification impact for a specific reactor design, in the full paper it will be discussed in some detail the typical case of the coolant reactivity effect in an innovative fast reactor concept. As for innovative fuel cycles, the extension of burn-ups for very long, once-through fuel cycles in fast neutron systems or the multiple recycle of TRU, also in fast neutron reactors, are both approaches intended to better exploit resources and to minimize the production or to drastically reduce the stocks of radioactive wastes. In the first case, the reactivity balance will change significantly during irradiation and should be monitored carefully, i.e. with an accurate uncertainty quantification. In the second case, the amount of TRU to be recycled, according to the objectives of the specific strategy, has an effect on crucial fuel cycle design parameters, also to be carefully assessed, both in terms of nominal values and of uncertainty quantifications. Examples related to the reactivity variation during the cycle and related to properties of the irradiated fuel, will be discussed in detail in the full paper.

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On the methodology to calculate covariance of estimated resonance parameters

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The majority of neutron induced reaction cross sections in evaluated data libraries are derived from nuclear reaction model. However, most of the models rely on parameters which are derived from an adjustment to experimental data. This is especially true for neutron cross sections in the resonance region. The resonance parameters are obtained from a least squares adjustment to the data and their covariances are in most cases obtained from conventional uncertainty propagation. In this contribution procedures to derive nuclear model parameters together with their covariance, in particular resonance parameters, from experimental data are discussed. Results obtained with Monte Carlo sampling, marginalization and generalized least squares adjustment are compared with results obtained from statistical theory, i.e. a full Bayesian probability analysis. Specific problems related to fitting of capture cross section data are addressed.

A novel Bayesian approach for nuclear data evaluation based on sampling[5]

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Several methods based on modeling exist for nuclear data evaluation. In this paper, we present the general Bayesian framework that allows to combine experimental data, knowledge of model parameter boundaries and model defects in a statistically consistent way. We propose a novel formulation of the prior which accounts for the deficiency of the applied physical model and conserves essential properties of the model, e.g., sum rules. The resulting posterior probability density function (pdf) has to be evaluated by means of Monte Carlo techniques. We point out a feasible way to approximately sample the posterior pdf in the case of computationally involved physical models. The new method is studied in a toy scenario with schematic experimental cross section data and a highly deficient linear model. The performance is compared to other methods in nuclear data evaluation such as the Empire-Kalmann-filtering technique (EKF), the Uniform Monte Carlo approach (UMC) and the Backward-Forward Monte Carlo approach (BFMC). The latter approaches are interpreted in the Bayesian framework and their underlying statistical assumptions are clearly pointed out. This comparison leads to the conclusion that model defects must be considered if the utilized physical model is not a perfect description of reality. We underpin this point by evaluating neutron-induced reaction cross section data of ^{181}Ta twice. In one evaluation model defects are considered, while in the second one they are neglected. The inherent consistency features of the presented procedure indicate that a consensus on using Bayesian statistics as standard framework for nuclear data evaluations can be reached.

[5]The work has been supported by the Austrian Academy of Sciences via the "Impulsprojekt_Schnabel".

Error analysis in the density functional theory approach to nuclear fission

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The mechanism of nuclear fission has been used successfully for several decades in practical applications such as energy production. However, our current understanding of most of these applications is essentially derived from semi-phenomenological models that are only remotely connected with the theory of nuclear forces, which explains the structure and reaction of an atomic nucleus. In addition, the free parameters of these semi-empirical models are often heavily tuned to fission data. Yet, in many areas of basic nuclear science where fission plays a major role, such as, e.g., the stability of superheavy elements, or the formation of elements in nuclear capture processes (fission recycling), experimental data is scarce at best, very often unavailable. A truly predictive theory of fission is thus needed. It poses formidable challenges, however, both conceptually, because of the need to follow the rules of quantum mechanics in strongly-interacting many-body systems, and in practice, because of the huge amount of computing power needed for simulations. A few years ago, the Lawrence Livermore National Laboratory has started such a comprehensive program on nuclear fission theory with leverage from large global US efforts such as the NUCLEI collaboration funded by the SciDAC 3 program from the US Department of Energy. Our framework to describe fission is nuclear energy density functional theory (DFT) coupled with large amplitude collective quantum dynamics. After giving a pedagogical overview of the DFT approach to the theory of fission, I will focus on very recent attempts to estimate theoretical errors by combining sensitivity analysis and Bayesian techniques.

Nuclear Data Uncertainties: Past, Present, and Future

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An historical overview is provided of the mathematical foundations of uncertainty quantification and the roles played in the more recent past by nuclear data uncertainties in nuclear data evaluations and nuclear applications. Significant advances that have established the mathematical framework for contemporary nuclear data evaluation methods, as well as the use of uncertainty information in nuclear data evaluation and nuclear applications, are described. This is followed by a brief examination of the current status concerning nuclear data evaluation methodology, covariance data generation, and the application of evaluated nuclear data uncertainties in contemporary nuclear technology. A few possible areas for future investigation of this subject are also suggested.

Delayed Neutron Activity Covariances

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The delayed neutron activity following fission is typically parameterized as a sum of 6 or 8 exponential terms. The ENDF/B library, for instance uses 6 terms, while JEFF uses 8. The neutrons are generated following the decay of a relatively small group of fission products, less than 50 and mainly neutron rich Br, Rb, I and Cs isotopes, for which the beta decay energy is larger than the neutron separation energy in the daughter nuclide. The delayed neutron activity can also be calculated by solving the corresponding Batemans equations using fission yields and decay data. This method can be incorporated into a Monte Carlo scheme to obtain covariance matrices for the delayed neutron activity as well as the parameters in the 6- or 8-group parameterizations. Recent results of these calculations will be presented. The calculated activities will be compared with the experimental Keepin values. Additionally, since measurements in the last 20 years have resulted in more precise decay, some valuable insights on the fission yields data and delayed nu-bars can be obtained. This work is part of an ongoing IAEA CRP on beta delayed neutrons.

Inventory Uncertainty Quantification using TENDL Covariance Data in Fispact-II

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The new inventory code Fispact-II provides predictions of inventory, radiological quantities and their uncertainties using nuclear data covariance information. Central to the method is a novel fast pathways search algorithm using directed graphs. The pathways output provides (1) an aid to identifying important reactions, (2) fast estimates of uncertainties, (3) reduced models that retain important nuclides and reactions for use in the code's monte-carlo sensitivity analysis module. Described are the methods that are being implemented for improving uncertainty predictions, quantification and propagation using the covariance data that the recent nuclear data libraries contain. In the TENDL library, above the upper energy of the resolved resonance range, a Monte Carlo method in which the covariance data come from uncertainties of the nuclear model calculations is used. The nuclear data files are read directly by Fispact-II without any further intermediate processing. Variance and covariance data are processed and used by Fispact-II to compute uncertainties in collapsed cross-sections, and these are in turn used to predict uncertainties in inventories and all derived radiological data.

Multiple-scattering corrections to measurements of the prompt fission neutron spectrum[6]

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The Chi-Nu project, conducted jointly by LANL and LLNL, aims to measure the shape of the prompt fission neutron spectrum (PFNS) for fission of ^{239}Pu induced by neutrons from 0.5 to 20 MeV with accuracies of 3-5% in the outgoing energy from 0.1 to 9 MeV and 15% from 9 to 12 MeV. In order to meet this goal, detailed Monte Carlo simulations are being used to assess the importance and effect of every component in the experimental configuration. As part of this effort, we have also simulated some past PFNS measurements to identify possible sources of systematic error. We find that multiple scattering plays an important role in the target geometry, collimators, and detector response and that past experiments probably underestimated the extent of this effect. This effort has highlighted the need for more complete and detailed reporting of the experimental environment and detector and target parameters.

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Covariance matrix evaluations for independent fission yields

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Recent needs for more accurate fission product yields include covariance informations to allow improved error estimations of engineering parameters used in applied calculations. The aim of this work is to investigate the possibility to generate reliable and complete uncertainties information on independent isotopic and isobaric fission yields. The procedures proposed are based on self-consistent empirical models for mass and isotopic yields. Mass yields covariance estimations are based on a convolution between the multi-Gaussian empirical model based on Brosas fission modes, which describe the pre-neutron mass yields, and the average prompt neutron multiplicity curve, better known as saw-tooth. Isotopic yields, instead, can be modelled by Wahls systematics, the Z_p-model for nuclear charge distribution. The covariance generation task has been approached using the Bayesian general least square method through the CONRAD code analysis tools, developed at CEA (Cadarache). Preliminary results on mass yields variance covariance matrix will be presented and discussed from physical grounds in the case of ^{235}U(n_{th}, f) reaction.

Uncertainty quantification in fission cross section and fragment distribution measurements at LANSCE

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Nuclear fission has been the subject of several experimental programs at LANSCE over the last few years. This is driven in part by the need for more precise nuclear data for applications, as well as by recent advances in the theoretical modeling of fission. Different aspects of the fission process have been studied; reaction cross sections, properties of fission fragments, and prompt neutron and gamma emission. In order for the measured data to be useful in nuclear data evaluations it is important to carefully quantify the associated uncertainties and correlations. The experimental work on measuring fission cross sections using a Time Projection Chamber (TPC) and ionization chambers will be presented here, and so will the work on fission fragment distributions using the SPIDER detector and Frisch-Gridded ionization chambers. The emphasis will be on how experimental uncertainties are estimated and how correlations are identified.

Quality quantification of evaluated cross section covariances

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One of the most important current stakes for nuclear cross section evaluations lies in their covariance matrix estimation. Presently, several methods used for code calibration (Bayesian, Backward-Forward Monte Carlo (BFMC), total Monte Carlo, scoring,...) are exploited for the covariance matrix estimation of evaluated nuclear cross sections. For all these methods the convergence rate of the covariance estimation is at least proportional to $1/\sqrt{n}$ (with n the sample size). However this convergence rate concerns each term of the covariance matrix. The convergence rate of the matrix estimation is thus lower. Moreover, for a given nucleus, according to the used method the covariance estimation can be different and according to the assumptions, with a same method, the estimation also could be different. Presently, these different estimations have not yet been compared and the quality quantification of the cross section covariance estimation remains an open subject. In order to solve this problem, we propose here a general and objective approach to quantify the quality of the covariance estimation of the evaluations. The first step consists in defining an objective criterion. The second step is the computation of the criterion. In this presentation several objective criteria (Kullback-Leibler and entropy distances) are proposed to compare the covariance matrix estimations. They are based on the distance to the real covariance matrix. The Kullback-Leibler distance and the entropy allow the comparison of the different methods or the different assumptions for the covariance matrix estimation. Moreover a method based on bootstrap is presented for the estimation of these criteria which can be applied with Bayesian, BFMC, total Monte Carlo and scoring approaches. The bootstrap is used for the Kullback-Leibler and entropy computation without the knowledge of the true covariance matrix. Thus, the full approach allows the comparison of the different covariance estimations independently of the method used to obtain them and without any additional code run. The full approach is illustrated on the ^{85}Rb nucleus evaluations. The results obtained on the ^{85}Rb nucleus are then used for a discussion on Bayesian, total Monte Carlo and scoring approaches for the covariance matrix estimation of the cross section evaluations.

Covariance Applications in Criticality Safety, Light Water Reactor Analysis, and Spent Fuel Characterization

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Significant advancement has been made during the last several years in providing nuclear data covariances for nuclear technology applications. These advancements include new covariance evaluations released in ENDF/B-VII.1 [1] for many important nuclides, as well as more approximate low fidelity uncertainty data [2] for nuclides without covariance evaluations in ENDF/B nuclear data files. Using these resources, a comprehensive library of covariance data [3] has been developed for the SCALE code system [4]. This covariance library – along with recent improvements in SCALE sensitivity/uncertainty (S/U) computation methods – provide the capability for realistic uncertainty analysis in many different applications [5].

Recently the SCALE nuclear data covariance library and S/U methodologies have been applied to a wide range of applications including (a) determination of uncertainties in multiplication factors of diverse types of critical experiments, (b) computation of uncertainties and correlations in calculated LWR assembly-homogenized two-group cross sections used in core simulators, and (c) uncertainties in spent fuel characteristics such as radionuclide concentrations and decay heat production. This presentation discusses recent results obtained for each of these types of applications.

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The current covariance evaluation based on the deterministic least-square approach in CNDC

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As well known, covariance is the hot issue in the modern nuclear data research. The deterministic least square (LS) approach is adopted to generate the covariance of nuclear reaction cross sections in China Nuclear Data Center (CNDC). Firstly, in order to achieve the covariance files for the nuclear data with plenty of measurements, a system named COVAC has been developed based on LS approach. In this system, the most difficult and time-consuming work is to extract the uncertainties and correlation values from experimental data to construct the experimental covariance Vexp. We specially make effort to study the different ways to deal with the data and errors belonging to various experimental techniques, such as activation and TOF, estimate and conclude some general error properties of every technique from our experimental evaluation so as to provide the basic reference to other experimental data evaluation whose original paper is hard to search or the description of experimental detail is too simple. Besides, some available tools including the SPCC (spline processing tool of experimental data) and CURVEFIT (polynomial processing tool of experimental data) are utilized to pre-analyze and handle the experimental data. The sensitive matrices F of various theoretical model parameters can be calculated by SEMAW, which is designed to incorporate the parameters in nuclear reaction codes: the Chinese UNF series, DWUCK and ECIS. Based on the research work above, the covariance of derived nuclear reaction cross sections (namely the recommended cross sections in CENDL) is obtained through integrating the experimental and theoretical information by LS error propagation approach. The output covariance is formatted in ENDF-6, the results are considered as the covariance in high fidelity. On the other hand, considering lots of nuclides and reactions lack of the experimental data like unstable nuclei and fission products, we are also trying to find a method to cover them. Recently, some changes are introduced in Vexp evaluation to determine this kind of covariance, the chief point is that their systematic errors can be obtained via applying the experimental data of the neighbored stable nuclides because we believe that systematic errors sourced from the detection equipment should be similar, and only the statistic error of unstable nuclei data is larger. We use

this method to produce the covariance in low fidelity. So far, the relevant approaches are suitable to the structure and fission nuclides in the fast neutron energy region. The whole procedure will be illuminated by some real evaluation of nuclides. Their benchmark tests are being performed in CNDC.

Use and impact of covariance data in a Japanese latest adjusted library ADJ2010 based on JENDL-4.0

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The current status of covariance applications to fast reactor analysis and design in Japan Atomic Energy Agency (JAEA) is summarized. In JAEA, the covariance data are mainly used for three purposes:

1. to quantify the uncertainty of nuclear core parameters,
2. to identify the important nuclides, reactions and energy ranges which are dominant to the uncertainty of core parameters,
3. to improve the accuracy of core design values by adopting the integral data such as the critical experiments and the power reactor operation data.

For the last purpose, the cross section adjustment based on the Bayesian theorem is used. After the release of JENDL-4.0, a development project of a new adjusted group-constant set ADJ2010 was started in 2010 and completed in 2013. ADJ2010 is based on the JENDL-4.0 data and finally combines 488 integral experimental data. ADJ2010 successfully improved the core design accuracy for a future power fast reactor. In addition, impact of the covariance data, especially for correlation factors, to the cross section adjustment is investigated by using parametric analysis.

Random sampling of correlated parameters a consistent solution for unfavorable condition

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As opposed to the deterministic approach, where only first few distribution moments (usually only the first two) are used in the uncertainty analysis, probabilistic approach requires knowledge about the entire distribution of the randomly sampled parameter(s). Nuclear data are usually given in the form of expected values and covariance matrices, i.e. the first two distribution moments. When restricted to this information only, normal distribution is the best possible guess. However, when inherently positive parameters (such as for example cross sections or resonance widths) with large relative uncertainties are in question, sampling according to normal distribution yields unphysical negative values. This problem can be circumvented by the use of lognormal distribution which has all the desired properties. While the sampling of individual (or independent) parameters is straightforward, random sampling of correlated parameters with large uncertainties is non-trivial multivariate lognormal distribution is to be employed. There are two possible solutions: the so-called correlated sampling method [1] which directly produces samples according to the multivariate lognormal distribution (or any combination of normal and lognormal distributions), or transformation of correlation coefficients [2] and distribution moments to log-space, covariance matrix diagonalization and sampling of individual uncorrelated linear combinations of logarithmized initial parameters.Though the latter seems to be more simple, the numerical complexity of both methods is comparable. Both methods are mathematically completely consistent and general, however numerical stability and convergence issues may arise at extremely unfavorable conditions, i.e. when dealing with a badly conditioned covariance matrix or extremely large relative uncertainties (order of 5000%!). The latter can be bypassed by weighted sampling, however this is only efficient for a very limited number of correlated parameters.

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Covariance analysis of the measured ^{40}Ca(n,tot) cross sections up to 20 MeV

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Accurate cross section data and covariance for ^{40}Ca(n,tot) reaction are particularly important for nuclear engineering and nuclear technique application because of its abundance in environment, but there is no any available related data up to now.

In this work, the recommended ^{40}Ca(n,tot) cross sections and corresponding covariance are based on experimental data evaluations. Considering experimental conditions and error sources, the collected measurements are analyzed in detail, and the reasonable recommendations are obtained. The errors are classified to systematic and statistic errors, evaluated reasonable association.

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