# Proceedings of the Workshop on Integral Experiment Covariance Data for Critical Safety Validation

9 - 11 March 2016
GRS Garching

GRS - 414

Gesellschaft für Anlagen-
und Reaktorsicherheit
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# Proceedings of the Workshop on Integral Experiment Covariance Data for Critical Safety Validation

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**Remark**

The authors are responsible for the content of the report.

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## Content

# 1 Introduction

For some time, attempts to quantify the statistical dependencies of critical experiments and to account for them properly in validation procedures were discussed in the literature by various groups. Besides the development of suitable methods especially the quality and modeling issues of the freely available experimental data are in the focus of current discussions, carried out for example in the *Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA)* of the OECD-NEA Nuclear Science Committee. The same committee compiles and publishes also the freely available experimental data in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments.* Most of these experiments were performed as series and might share parts of experimental setups leading to correlated results. The quality of the determination of these correlations and the underlying covariance data depend strongly on the quality of the documentation of experiments.

The meeting entitled *Workshop on Integral Experiment Covariance Data for Criticality Safety Validation* was organized by *the Gesellschaft für Anlagen- und Reaktorsicherheit* (GRS) and took place from 9 to 11 March 2016 in Garching, Germany. For the first time it offered the participants a separate meeting on the topic of generation and usage of covariance data and thus a detailed exchange of knowledge.

The aim of the workshop was to present various methods and approaches and the resulting implications for future research developments. For that, a total of 17 participants from 10 organizations discussed the topics and presented their current state of scientific knowledge in 15 presentations.

For the Proceedings at hand, each contributor summarized his talk and if necessary referenced already published relevant work. For more detailed information on the presentations, the contact data of all participants is provided in chapter 3. Apart from this proceeding, the participants of this workshop collaborate on a more detailed report on the current state of scientific knowledge to be published later on.

# 2 Proceedings

## 2.1 A Review of Current Literature Regarding Critical Experiment Correlations

William J. Marshall,
Oak Ridge National Laboratory, U.S.A.

A series of publications are available in the literature currently discussing different methods of determining correlations among critical experiment correlations. At least four different methodologies have been proposed, including both deterministic and stochastic approaches. A range of methods have also been outlined for incorporating the covariance data in validation and data adjustment applications. In general, incorporation of covariance data increases the uncertainty of biases determined from validation because of the effective reduction in the available, independent data. A more detailed list of references used will be generated in the future.

[1] T. T. Ivanova, M. N. Nikolaev, K. F. Raskach, E. V. Rozhikhin, A. M. Tsiboulia , “Influence of the Correlations of Experimental Uncertainties on Criticality Prediction”, Nuclear Science and Engineering Vol. 145, No.1,pp. 97-104. September 2003.

[2] T.T. Ivanova et al., “Towards validation of criticality calculations for systems with MOX powders”, Annals of Nuclear Energy, 36, pp. 305–309, 2009.

[3] Working Party on International Nuclear Data Evaluation Co-operation of the NEA Nuclear Science Committee, “Methods and Issues for the Combined Use of Integral Experiments and Covariance Data”, NEA/NSC/WPEC/DOC(2013)445.

[4] T. Ivanova, E. Ivanov, G. E. Bianchi, “Establishment of Correlations for Some Critical and Reactor Physics Experiments”, Nuclear Science and Engineering, Vol. 178, No. 3, pp. 311-325, November 2014.

[5] O. Buss., A. Hoefer, J.C. Neuber, „Hierarchical Monte Carlo approachto bias estimation for criticality safety calculations", Proc. Physics of Reactors International Conference (PHYSOR2010). Pittsburgh, Pennsilvania, USA. 2010.

[6] V. Sobes, B.T. Rearden, D.E. Mueller, W.J. Marshall, J.M. Scaglione, and M.E. Dunn, "Upper Subcritical Calculations Based on Correlated Data" ", Proc. Int. Conf. on Nuclear Criticality Safety, ICNC 2015, Charlotte, NC, USA, 13-17 Sept.2015.

## 2.2 PSI CSE methodology status and prospects for its further upgrading

Alexander Vasiliev,
Paul Scherrer Institut, Switzerland

The PSI methodology for criticality safety evaluations (CSE) is based on the use of MCNP(X) code and its validation against relevant critical benchmark experiments from the ICSBEP Handbook [1]. The main areas being considered currently as requiring improvements include [2]:

- Taking into account the benchmark correlations into the definition of keff Upper Subcritical Limit (USL) and
- Assessment of physical similarity between an application case and the benchmarks from the validation suite (benchmarks representability).

For that purposes the recently developed at PSI tools – MTUQ (Manufacturing and Technological Uncertainty Quantification) [3] and NUSS-RF (Nuclear data Uncertainty Stochastic Sampling) [4,5,6], operational with MCNP(X) code and utilizing the Monte Carlo sampling technique, are planned to be integrated in CSE(+burnup credit) [2] and the details of these ideas were discussed at the presentation. The new calculation capabilities support a general trend in the CSE philosophy which is a gradual transition towards explicit evaluation of an application case (and benchmarks) keff uncertainties. In this relation a revision of the USL definition might be required in order to avoid excessive conservatism and double counting the same sources of calculation uncertainties [1]. Finally, a need for application of the data assimilation techniques (i.e., 'adjusting' the general- purpose nuclear data variance-covariance matrices for a specific area of applicability) in combination with the validation studies was acknowledged.

[1] A. Vasiliev, E. Kolbe, M.A. Zimmermann. Towards the Development of Upper Subcriticality Limits on the Basis of Benchmark Criticality Calculations. Ann. Nucl. Energy, 35, 1831-1841 (2008).

[2] A. Vasiliev, D. Rochman, T. Zhu, M. Pecchia, H. Ferroukhi, A. Pautz. Towards Application of Neutron Cross-Section Uncertainty Propagation Capability in the Criticality Safety Methodology. Proc. Int. Conf. Nuclear Criticality Safety, ICNC 2015, Charlotte, NC, USA, September 13-17, 2015.

[3] M. Pecchia, A. Vasiliev, O. Leray, H. Ferroukhi, A. Pautz. Advanced calculation methodology for manufacturing and technological parameters' uncertainties propagation at arbitrary level of lattice elements grouping. Journal of Nuclear Science and Technology, Vol. 52:7-8, pp. 1084-1092, (2015)

[4] T. Zhu, A. Vasiliev, H. Ferroukhi, A. Pautz. NUSS: A tool for propagating multigroup nuclear data covariances in pointwise ACE-formatted nuclear data using stochastic sampling method. Ann. Nucl. Energy, Vol. 75, pp. 713-722 (2015).

[5] T. Zhu, A. Vasiliev, D. Rochman, H. Ferroukhi, A. Pautz. Testing the Sampling-based NUSS-RF Tool for the Nuclear Data Related Global Sensitivity Analysis with Monte Carlo Neutronics Calculations. To be published in Nucl. Sci. Eng., (accepted in March 2016).

[6] D. Rochman, A. Vasiliev, H. Ferroukhi, T. Zhu, S.C. van der Marck, A.J. Koning. Nuclear data uncertainty for criticality-safety: Monte Carlo vs. linear perturbation. Ann. Nucl. Energy, Vol. 92, pp. 150-160 (2016).

## 2.3 ANSWERS Uncertainty Modeling and UACSA Phase IV Benchmark

Christopher Baker,
Amec Foster Wheeler, U.K.

The uncertainty quantification methods utilised at ANSWERS was presented together with an overview of our existing methods to categorise criticality safety runs for our customers. This was followed by the strategy we used for the UACSA Phase IV benchmarks together with the correlation matrices produced for this for scenarios A and E. This was applied to an application case which folded in the biases and their associated uncertainties produced from validation cases. When we assume that the experimental configurations from the validation cases are correlated, we obtain a more conservative estimate on the uncertainty on the bias.

[1] Christopher Baker, Paul N. Smith, Robert Mason, Max Shepherd, Simon Richards, Richard Hiles, Ray Perry, Dave Hanlon, Geoff Dobson, “Calculating Uncertainty on K-Effective with MONK10”, Proc. ANS NCSD 2013 Meeting “Criticality Safety in the Modern Era: Raising the Bar.” Wilmington, NC, September 2013.

## 2.4 Technical Overview SUnCISTT

Fabian Sommer,
Gesellschaft für Anlagen- und Reaktorsicherheit, Germany

SUnCISTT (Sensitivity and Uncertainty in Criticality Inventory and Source Term Tool) provides an abstract interface to combine well established codes for burnup (e.g. Orest, Helios, Triton, Kenorest, Serpent) and criticality calculations (e.g. KENO (SCALE), NEWT, MCNP) with an uncertainty and sensitivity analysis based on Monte-Carlo sampling utilizing statistics procedures, ROOT and Python [1,2]. It needs a template file of the code with keywords, a list of varied numeric input parameters, a mapping file to map between the numerical values and the keywords and an optional self-defined math model to process the parameters (in Python). SUnCISTT resolves all dependencies between parameters, replaces the keywords, creates the input files, runs all individual calculations, extracts and collects relevant results from the individual output files and saves these results as ROOT TTree and ASCII file. From these compact result tables an uncertainty analysis of the calculated values (e.g. $k_{eff}$, EALF, number densities) a sensitivity measure (Pearson correlation) of the calculated values on the varied parameters and the correlations between different experiments due to shared variation of system parameters can be calculated, including error estimates on the correlation coefficients [3]. SUnCISTT can also be applied to any code outside the field of nuclear criticality safety, using ASCII input- and output files [1].

[1] M. Behler, M. Bock, F. Rowold, M. Stuke, "SUnCISTT - A Generic Code Interface for Uncertainty and Sensitivity Analysis", Proc. PSAM12, 2014.

[2] M. Bock and M. Stuke, "Determination of Correlations Among Benchmark Experiments by Monte Carlo Sampling Techniques", Proc. ANS NCSD 2013 Meeting "Criticality Safety in the Modern Era: Raising the Bar." Wilmington, NC, September 2013.

[3] E. Peters, F. Sommer, M. Stuke, " Modeling of critical experiments and its impact on integral covariance matrices and correlation coefficients Annals of Nuclear Energy (2016), pp. 355-362, doi:10.1016/j.anucene.2016.02.011, [arXiv:1602.04038 [physics.data-an]].

## 2.5 Recent developments for the UACSA benchmark on LCT-007 and LCT-039

William.J. Marshall,
Oak Ridge National Laboratory, USA

The correlation coefficient matrix for all cases included in the WPNCS UACSA benchmark from July, 2015, has been determined. There are slight differences for parameters among the scenarios, but for Scenario E all coefficients are generated using 300 realizations for each experiment and each calculation converged to a calculational uncertainty of 0.00010 Δk. The results indicate that the correlation coefficients are well converged within about 100 realizations, and that the coefficients increase with lower Monte Carlo uncertainties on the individual case calculations. An initial estimate of the uncertainty coefficient was generated for one case and may on the order of 10% for a correlation coefficient of 0.3. Overall, these results are in good agreement with results generated by other WPNCS UACSA benchmark Phase IV participants.

[1] W. J. Marshall and B. T. Rearden, "Determination of critical experiment correlations using the Sampler sequence within SCALE 6.2", Proc. Int. Conf. on Nuclear Criticality Safety, ICNC 2015, Charlotte, NC, USA, 13-17 Sept.2015.

## 2.6 Playing around with MC sampling of Critical Experiments

Maik Stuke,
Gesellschaft für Anlagen- und Reaktorsicherheit, Germany

Comparing covariance or correlation matrices resulting from the same set of experimental data but determined by different evaluators with different methods can become non-trivial if further steps within the analysis are not specified well, e.g.

- Interpretation of given experimental data might vary for each evaluator leading to different modelling assumptions and thus to different covariance's and correlation coefficients [1].
- Following a Monte Carlo Sampling approach for the determination of the correlation coefficients one has to choose suitable parameters for e.g. for σ(MC) of $k_{eff}$ or the number of samples.

A better approach to compare the results for an analysis including correlated data might be to compare the resulting bias for a given application case and a given covariance matrix. In this way the different methods used by different evaluators could be compared as the end effect on e.g. the upper safety criticality limits.

[1] E. Peters, F. Sommer and M. Stuke, ``Modeling of critical experiments and its impact on integral covariance matrices and correlation coefficients,' Annals of Nuclear Energy (2016), pp. 355-362, doi:10.1016/j.anucene.2016.02.011, [arXiv:1602.04038 [physics.data-an]].

## 2.7 Approach and issues of covariance matrix establishment for systems with variable spectra

Evgeny Ivanov, Institut de Radioprotection et de Sûreté Nucléaire

Integral experiments (IEs) data is an essential part of a validation process. The information contained in the available IEs data can be characterized quantifying benchmarks uncertainties and relevant covariance matrices. Both firm evaluation of uncertainties and establishment of their correlations are crucial for the confidence of validation. Basing on its background IRSN considered one series of the benchmarks with parametrically varied spectra (BFS-MOX series). The covariance matrix for BFS-MOX series has been established, analyzed and recommended to be included in the ICSBEP Handbook.

## 2.8 Propagation of rod position uncertainty in lattices: an issue to correctly assess uncertainties of associated benchmarks and their correlations

Nicolas Leclaire,
Institut de Radioprotection et de Sûreté Nucléaire, France

With the growth of methodologies based on the use of correlation matrices in support to the GLLSM method, the propagation of experimental uncertainties in terms of $\Delta k_{eff}$ has become a paramount issue. And it is particularly acute for tightly packed lattices of rods [1], corresponding to a low moderation ratio. The work conducted by IRSN consisted in identifying the different sources of rod position uncertainties for rods installed in grids and in propagating them in terms of $\Delta k_{eff}$ [2]. Diverse methodologies were tested using either “traditional” practices (expansion and reduction of the size of regular lattices, extreme lattice bounds technique), Monte Carlo sampling with the MORET 5 code [3] and the PROMETHEE workbench [4] dealing with uncorrelated positions of rods, geometry perturbation calculation using the URAN card of the MCNP6 code. Through the comparison with repeatability/reproducibility experiments for various IRSN programs, it was possible to show that “traditional” methods overestimated the rod positioning uncertainty for low moderated lattices, which was not the case for the Monte Carlo sampling or for the geometry perturbation with URAN. Indeed, these two methods predicted rather well the rod position uncertainty. However, for the optimum moderation ratio, quite consistent results were obtained whatever the method.

[1] International Handbook of Evaluated Criticality Safety Benchmark Experiments, OECD, NEA, September 2015

[2] N. Leclaire, EGUACSA 2014/08 – Evaluation of Rods’ Position Uncertainty

[3] B. Cochet et al., ‘”Capabilities overview of the MORET 5 Monte Carlo code”, Annals of Nuclear energy, August 2015, Vol. 82

[4] Yann Richet et al.,”Second level criticality modelling: beyond k-effective calculation, nuclear criticality safety begins…”, Proc. Int. Conf. on Nuclear Criticality Safety, ICNC 2015, Charlotte, NC, USA, 13-17 Sept.2015.

## 2.9 From covariances to safety margins: data, methods and tools

Axel Hoefer,
AREVA, Germany

The impact of a set of benchmark experiments w.r.t. the prediction of an integral observable (application case) is determined by different kinds of covariances due to nuclear data uncertainties and due to system parameter uncertainties:

- Covariances between application case variables and benchmark variables. These covariances define how much the prediction uncertainty can be reduced by taking into account benchmark data.
- Covariances between variables of different benchmarks experiments. These covariances reduce the amount of information from benchmark experiments for the prediction of the application case.

Hence, a reasonable validation procedure has to take into account all of these covariances within a consistent statistical model. Within the perturbation theory framework this is achieved by the GLLS procedure, within the Monte Carlo framework by the MOCABA procedure. Mathematically, MOCABA is the non-perturbative generalization of GLLS.

[1] O. Buss., A. Hoefer, J.C. Neuber, „Hierarchical Monte Carlo approachto bias estimation for criticality safety calculations", Proc. Physics of Reactors International Conference (PHYSOR2010). Pittsburgh, Pennsilvania, USA. 2010.

[2] A. Hoefer, O. Buss, M. Hennebach, M. Schmid and D. Porsch,"MOCABA: a general Monte Carlo-Bayes procedure for improved predictions of integral functions of nuclear data," Annals of Nuclear Energy (2015) pp. 514-521, doi:10.1016/ j.anucene.2014.11.038, [arXiv:1411.3172 [nucl-th]].

## 2.10 Generation of Integral Experiment Covariances for DICE

Tatiana Ivanova, Ian Hill,
OECD-NEA

The NEA Database for the International Criticality Safety Benchmark Evaluation Project (DICE) contains correlation coefficient data of benchmark keff uncertainties (or experimental covariances) and sensitivity-based correlations. Currently work is going on to extend the collection of experimental covariances. Thus, low-fidelity covariance data have been generated for about 600 LEU-COMP-THERM configurations available in the ICSBEP Handbook. A set of rules that help quantifying the shared uncertainty between cases, within evaluations, is being established in the “Rules” document. An excel spreadsheet has been created to facilitate the generation of covariance matrices from the uncertainties contained in legacy evaluations. The presentation provides status of the covariances existing in DICE and describes how new the matrices have been generated.

## 2.11 Identification, accounting for and documentation of local and global correlations and their effects in an IRPhEP Handbook evaluation

Dennis Mennerdahl,
E. Mennerdahl Systems, Sweden

A single, accurately specified benchmark, with no uncertainty and identical to the application, is the ideal standard for validation. Global and local (affect all or sub-groups of benchmarks, respectively) correlations should be determined and specified individually for each potential error source. An ongoing IRPhE handbook evaluation demonstrates how an accurate deterministic relationship (boron concentration versus temperature), when achievable, is preferred over a statistic compilation of data. The measured critical water heights versus temperature deviate very little from a non-linear regression fit, indicating almost full correlation, with small random effect uncertainties. Correlations influence biases and bias uncertainties (both random effect and systematic effect) as well as values with no estimated bias and uncertainty (human factor). Evaluations of covariance's need to be documented transparently to support understanding and reduction of remaining biases and bias uncertainties as well as identification of additional error sources. The human factor, in all steps, needs to be considered, and possibly quantified, in a complete evaluation of potential error sources and their effects on the measured results.

## 2.12 Validation of criticality calculations including geometrical and nuclear data uncertainties

Maksym Chernykh, Sven Tittelbach, Jens C. Neuber,
Wissenschaftlich-Technische Ingenieurberatung, Germany

The presentation describes the methodology for validation of criticality calculations based on DIN 25478, Supplement 1. A total of 132 critical LEU-COMP-THERM (LCT) benchmark configurations from ICSBEP Handbook were analysed. For the evaluation of material and geometrical uncertainties the Monte Carlo analysis was implemented. The benchmark uncertainties due to nuclear data were evaluated using TSUNAMI from SCALE 6.1 code package.

The covariance and correlation matrices for the benchmark experiments due to geometrical and nuclear data uncertainties were generated and the impact of these uncertainties on the criticality safety assessment for some representative transport and storage cask application was investigated. The results show that the geometrical uncertainties of the analysed benchmark experiments can be neglected compared to the nuclear data uncertainties.

Additionally, the analytical toy benchmark model from the UACSA Benchmark Phase IV was analysed applying the same methodology. The results show a very good agreement with other methodologies.

## 2.13 ORNL results for correlations in LCT-042

William J. Marshall,
Oak Ridge National Laboratory, USA

The correlation coefficient matrix for the 7 cases in LCT-042 was generated using the Monte Carlo sampling approach. The experiments were performed at Pacific Northwest Laboratory and included three arrays of fuel rods with poison panels located between the arrays. Each case has a unique poison panel material, contributing independent uncertainty to each case. The fuel rod pitch is assumed to be constant between all rods in all cases, which is the same as the treatment in Scenario A in the WPNCS UACSA benchmark. The correlation coefficients range from 0.78 – 0.85, which clearly shows the impact of independent uncertainty components. Also, a crude study on the effect of the pin pitch assumption on the correlation coefficients indicates that it is the controlling uncertainty in determining the correlation coefficients.

[1] W.J. Marshall and B.T. Rearden, "Determination of Experimental Correlations Using the Sampler Sequence Within SCALE 6.2," Trans. Am. Nucl. Soc. 111 (2014).

## 2.14 The Use of Maximum Likelihood Estimation for Calculating the Bias

Christopher Baker,
Amec Foster Wheeler, U.K.

This presentation aimed to look at bias estimation without the need to carry out any sampling through the use of Maximum Likelihood Estimators (MLEs) and showed our initial work in this area. For this, we assume that the underlying data has a normal distribution and we can then estimate the bias based on pre-existing data without any considerable computational expense. The method can be used to validate experiment selection based on engineering judgement and provides a framework on estimating overall bias as well as separating out the contributions from individual cases.

## 2.15 Impact of different distribution functions of parameters describing LCT-006, 035, and 062

Elisabeth Peters,
Gesellschaft für Anlagen- und Reaktorsicherheit, Germany

In the presentation the impact of different distribution functions for varied parameters was analyzed using a set of nine LEU-COMP-THERM (LCT) experiments. Following the Monte Carlo sampling approach the effective neutron multiplication factors keff were calculated along with the corresponding covariance and correlation coefficients utilizing SUnCISTT and SCALE. It was found that the calculated keff values for the experiment series LCT-06 and -35 were underestimated by SCALE while for LCT-62 they were overestimated. Furthermore, considering the three cases, all parameters are either normally or uniform distributed or a mixture of both, the correlation coefficients varied by up to 20%. While the variations of the correlation coefficients had only a minor effect in a Bayesian updating process, updating using experiments with under- or overestimated keff values may have led to wrong bias determination. Benchmark experiments as well as the application case must be chosen and analyzed carefully, since hidden experimental and/or calculation systematics may lead to misleading results [1].

[1] Peters, E., Sommer, F., Stuke, M.: The Bumpy Road to Code Validation Including Correlations, accepted for Proceedings PHYSOR2016, 2016.

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