# Creation of a Database of Uncertainties for ICSBEP Handbook and Tool for Covariance Generation

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**Abstract** – The creation of a database of uncertainties for criticality experiment benchmarks is under construction and intended to be incorporated into a future version of the database for ICSBEP, DICE. As a first step, Section 2 and 3.1 data have been extracted from ICSBEP benchmark evaluations and homogenized in a manner that allows searching and trending uncertainties across evaluations. One of the primary objectives of building such a database is to facilitate creation of covariance matrices between experimental uncertainties, as often, only the diagonal term has been evaluated leading to cases being treated as independent during uncertainty analysis. This assumption does not reflect a best estimate. The database-features lower the effort required to create covariance's, so analysts can focus on estimating whether uncertainties are shared between cases, rather than the mechanical aspects of uncertainty extraction and matrix generation. Now users can quickly create transparent estimates of covariance. Using the sheet an attempt has been made to read the evaluations and then provide an estimate of the covariance by estimating which uncertainty components are shared between cases. While it is difficult to evaluate the 'correctness' of the generated covariance's, the paper has run the over 500 of LCT cases with experimental covariance, through a generalized least squares tool, TSURFER, both with experimental covariance's and without and the results are analyzed. Further work is required in the area of testing the impact on real world applications.

## I. INTRODUCTION

This paper presents work done to create a database of uncertainties for International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [1]. The Handbook contains nearly 5000 experimentally based benchmark models and each has an associated uncertainty in  $k_{\rm eff}$  that serves as a quantitative indicator of the accuracy. Uncertainties include both those associated with the measurements, as well as uncertainties from modelling owing to imperfect knowledge of the exact compositions and geometries used in the experiment.

With such a large set of benchmarks uncertainties it is possible to analyse the dataset in order to identify trends in uncertainty analysis, for example scrutinizing the average uncertainty for fuel impurities. Examining outliers could lead to identifying errors, or assist evaluators in making reasonable estimations in the absence of information.

Furthermore, creating such a database of uncertainty information presents a unique opportunity to structure the data in a way that facilitates the generation of covariance matrices between experimental benchmark models. And while the uncertainty information for ICSBEP benchmarks are well characterized, covariance is sparse. A similar situation of uncertainties without covariance was faced by the nuclear data community in the 1970's and is still actively being worked on today. Recently a web tool [2] was created that can generate nuclear data covariance matrices by assigning which EXFOR uncertainty components are shared between data points. With a similar concept in mind, the uncertainty extraction and corresponding database have been engineered to have similar functionality, allowing users to identify which uncertainties are shared between experiments, to estimate the covariance.

Uncertainty information will ultimately be made accessible to users via the Database for ICSBEP (DICE) [3], supplementing the limited correlation data already generated and available [4]. With the covariance data, the degree of shared uncertainty between the cases can be estimated, assisting the user to better identify a suitable set of benchmarks for validation. Ultimately, the purpose of making the tool is to improve validation for a variety of applications. Like estimates of nuclear data covariance, any estimate of the covariance should be based upon the best available information and not artificially made to agree with a particular applications.

Finally, while it is readily accepted that the existing assumption of no correlations between cases within an evaluation is certainly not true, it is difficult to justify the quality of a particular choice. After creating covariance's using the database and tools, we have attempted to show the impact by comparing, generalized least squares adjustment results with and without experimental covariance's using TSURFER[5].

# **II. DATABASE CONSTRUCTION**

#### 1. Data extraction

In the ICSBEP handbook, criticality benchmark experiments are categorized according to fissile material, physical form, neutron energy causing fission and a threedigit numerical identifier. In this work, benchmark experimental uncertainties from those experiments identified as LEU-COMP-THERM and HEU-MET-FAST was extracted and subsequently sample covariance matrices quantifying shared uncertainty between the benchmark cases have been generated.

The first step in populating the database is to extract all of the Section 2 uncertainties [6] from the benchmark evaluations. Some evaluations provide detailed uncertainty estimates only for a subset of the cases, so part of the work is to ensure that the proper representative case is matched with all cases for which it is intended to serve as the uncertainty assessment. Furthermore, many evaluations do not have a simple summary table, so care must be taken to extract the correct uncertainty values, requiring familiarity with ICSBEP evaluations and formats. Next, model simplification uncertainties from Section 3.1 and total benchmark model uncertainties from Section 3.5 are extracted. With this information, the excel sheet computes the sum of individual uncertainties in quadrature and compares to the total uncertainty from Section 3.5, and large disagreements indicate if one of the components has been missed during the extraction process.

During extraction the uncertainties are converted to pcm, as standard units of uncertainty are not required in the existing ICSBEP format guide. Also, the uncertainties are assigned categorization by type, examples include 'geometry', 'composition', 'experiment', and 'modeling'. The classification allows users to quickly assess the dominant types of uncertainties in evaluations; also it allows for anomalies to be identified. Furthermore, a separate categorization is done corresponding to the physical region that contributes to the uncertainty, examples include, 'fuel', 'cladding', 'moderator', 'core', etc. Searches can then be performed using the categorizations, such as returning all 'fuel' + 'composition' uncertainties for each LCT case.

Next, the percentage variance that each uncertainty term contributes is computed and the most influential terms are identified. A criterion is applied to identify terms that correspond to at least 90% of the total variance; specifically 90% of the sum of the individual variances (rather than comparing to Section 3.5). Users then have the opportunity to assign whether these top contributors are shared between cases, allowing for the total shared uncertainty between the two cases to be computed. Currently the sheet allows only for covariances between cases within evaluations, although it is recognized that in the future, functionality for inter evaluation case level correlations will be needed.

Evalle	Caseld TypeSet	RegionSet	Description Partial or	TO' Basi Uni +c Ur -o Urio-keff	(pcm) keft	(pcm) Assun	ption				
LEU-COMP-THERM-000	1 Composition	Fuel	Enrichment (± 0.01 wt.%)		100	90	11.11	11.11	0.14	0.63	0.63
LEU-COMP-THERM-000	1 Ge	mbas coluto	Fuel Diameter (± 0.0127 cm)		100	80	11.11	11.11	0.14	0.14	0.77
LEU-COMP-THERM-000	1 Ge pormalius	unck the formulas	Fuel Length (± 0.127 cm)		70	0	5.44	5.44	0.07	0.14	0.92
LEU-COMP-THERM-000	1 Ge		Clad Diameter (± 0.00127 cm)		0	10	0.11	0.11	0.00	0.07	0.99
LEU-COMP-THERM-000	1 Geometry	Core	Pitch (± 0.0076 cm)		140	210	49.00	49.00	0.63	0.01	1.00
LEU-COMP-THERM-000	1 Composition	Fuel	Uranium Mass (-0.81 g and			10	1.00	1.00	0.01	0.00	1.00
LEU-COMP-THERM-000	1 Measurement	Coolant/Moderator/Reflector	Temperature	et to be filled by "Total" in the		5	0.03	0.03	0.00	0.00	1.00
LEU-COMP-THERM-000	1 Geometry	Core	Cluster Separation	tomor each cases to normality.		0	0.00	0.00	0.00	0.00	1.00
LEU-COMP-THERM-000	1 TOTAL	TOTAL	Total	K the formulas		300	0.00	0.00	0.00	0.00	0.00
LEU-COMP-THERM-000	2 Composition	Fuel	Enrichment (± 0.01 wt.%)		100	2 90	11/1	11.11	0.14	0.63	63 1
LEU-COMP-THERM-000	2 Geometry	Fuel					11 1	11-11	0.14	0.14	.77 1
LEU-COMP-THERM-000	2 Geometry	Fuel									.92 (
LEU-COMP-THERM-000	2 Geometry	Clad		Uncertainty	z ncr	n	Per	cent	аде с	of 1	.99
LEU-COMP-THERM-000	2 Geometry	Core		oncertainty	Pen		1.01	centa	aget	7	.00
LEU-COMP-THERM-000	2 Composition	Fuel					Tot	al Va	rian	ce	.00
LEU-COMP-THERM-000	2 Measurement	Core					100	arva	Ian		.00
LEU-COMP-THERM-000	2 Geometry	Core					0.00	0.00	0.00	0.00	.00
LEU-COMP-THERM-000	2 TOTAL	TOTAL									
LEU-COMP-THERM-000	3 Composition	Fuel					Reo	rdere	d Fr	actio	in 🗌
LEU-COMP-THERM-000	3 Geometry	Fuel					Reor	uere		actio	
LEU-COMP-THERM-000	3 Geometry	Fuel					of Si	ımm	ed V	ariar	ice
LEU-COMP-THERM-000	3 Geometry	Clad					01.01		cu v	uriur	ice
LEU-COMP-THERM-000	3 Geometry	Core	in menta or on on only		240		49.00	49.00	0.63	0.01	1.00
LEU-COMP-THERM-000	3 Composition	Fuel	Uranium Mass (-0.81 g and +0.43	1 g)	30	10	1.00	1.00	0.01	0.00	1.00
LEU-COMP-THERM-000	3 Measurement	Core	Temperature		5	5	0.03	0.03	0.00	0.00	1.00
LEU-COMP-THERM-000	3 Geometry	Core	Cluster Separation		0	0	0.00	0.00	0.00	0.00	1.00
LEU-COMP-THERM-000	3 TOTAL	TOTAL	Total		300	300	0.00	0.00	0.00	0.00	0.00
LEU-COMP-THERM-000	4 Composition	Fuel	Enrichment (± 0.01 wt.%)		100	90	11.11	11.11	0.14	0.63	0.63
LEU-COMP-THERM-000	4 Geometry	Fuel	Fuel Diameter (± 0.0127 cm)		100	80	11.11	11.11	0.14	0.14	0.77 1
LEU-COMP-THERM-000	4 Geometry	Fuel	Fuel Length (± 0.127 cm)		70	0	5.44	5.45	0.07	0.14	0.92 (
LEU-COMP-THERM-000	4 Geometry	Clad	Clad Diameter (± 0.00127 cm)		0	10	0.11	0.11	0.00	0.07	0.99
LEU-COMP-THERM-000	4 Geometry	Core	Pitch (± 0.0076 cm)		140	210	49.00	49.00	0.63	0.01	1.00
LEU-COMP-THERM-000	4 Composition	Fuel	Uranium Mass (-0.81 g and +0.43	1 g)	30	10	1.00	1.00	0.01	0.00	1.00
LEU-COMP-THERM-000	4 Measurement	Core	Temperature		5	5	0.03	0.03	0.00	0.00	1.00
LEU-COMP-THERM-000	4 Geometry	Core	Cluster Separation		0	0	0.00	0.00	0.00	0.00	1.00
LEU-COMP-THERM-000	4 TOTAL	TOTAL	Total		300	300	0.00	0.00	0.00	0.00	0.00

Fig. 1. Example of Uncertainty Data Extraction Sheet.

#### 2. Covariance matrix sheet

Once the top uncertainty terms are identified a new worksheet is automatically populated with the top terms. The intent is to isolate dominate terms so that judgement can be focused on the key uncertainties, making correlation assignment more efficient. An example of the sheet is shown in Fig. 2., where the five uncertainties contributing 90% of the variance are listed in order from the largest contributor to the smallest. An evaluator or user of the spreadsheet can then assign the fraction of fuel diameter uncertainty that is shared between the cases within an evaluation, in the example shown the burden is to provide five assignments of the degree of shared uncertainty. Some judgements are easier than others. For example, if the same fuel is used, and the system remains either over or under moderated then the fraction shared from fuel diameter is likely to be high. Once this assignment is performed for each of the top terms, equation 1 is used to compute the shared uncertainty between the cases, by summing all of the shared uncertainty components, *i*, between case A ( $\sigma_{A,i}$ ) and case B ( $\sigma_{B,i}$ ) and dividing by the total uncertainty for each case,  $\sigma_{A,T}$  and  $\sigma_{B,T}$ . The user is supplies judgement of whether the uncertainty is shared or not  $\rho_{AiBi}$ .

$$\rho_{A,B} = \frac{\sum_{i} \sigma_{A,i} \rho_{Ai,Bi} \sigma_{B,i}}{\sigma_{A,T} \sigma_{B,T}}$$
(Eq. 1)

The correlation matrix, is given in the spreadsheet, because it is easier for to interpret than the covariance matrix, however the covariance matrix,  $\mathbf{V}$ , often needs to be formed for uncertainty analysis; this is easily done as it is the numerator of equation 1.

The spreadsheet also computes the average of calculated over experimental values [C/E] with a simple average, as well as with a weighted average using the full inverse of the experimental covariance matrix, see equation below.

$$GLSMean = (X'V^{-1}X)^{-1}X'V^{-1}[\frac{c}{E}]$$
 (Eq. 2)

Where X is a 1d matrix of ones of the same length as the number of calculated over experimental [C/E] values.

Users receive quick feedback of the impact of assigned correlations. But the real strength of the sheet is transparency. If a user has reason to change the amount of shared uncertainty of an uncertainty component only a single number need be changed. The worksheet is updated automatically and it is simple to copy and paste the newly generated experimental correlation matrix into application codes. Information flow can be easily tracked in the excel sheets.

1	А	В	С	D	E	F	L	М	N	0	Р	Q	R	S	Т	U
1	Comments:							Correlations(Betwee	All Cases							
2								Pitch (± 0.0076 cm)	0.99							
3	Average C/E							Fuel Diameter (± 0.0	0.99							
4	0.99911883							Enrichment (± 0.01 w	0.99							
5								Fuel Length (± 0.127	0.99							
6	Weighted Avera	age C/	E					Cluster Separation	0.2							
7	_	-						Free	0							
8								Free	0							
9	GLS Average C/	E						Free	0							
10	0.99437309							Free	0							
13								Uncertainties(pcm)	Case1	Case2	Case3	Case4	Case5	Case6	Case7	Case8
14								Pitch (± 0.0076 cm)	210	210	210	210	210	210	210	210
15								Fuel Diameter (± 0.0)	100	100	100	100	100	100	100	100
16								Enrichment (± 0.01 w	100	100	100	100	100	100	100	100
17								Fuel Length (± 0.127	70	70	70	70	70	70	70	70
18								Cluster Separation	0	40	50	50	50	50	90	40
19								Free	0	0	0	0	0	0	0	0
20								Free	0	0	0	0	0	0	0	0
21								Free	0	0	0	0	0	0	0	0
22								Free	0	0	0	0	0	0	0	0
23								Free	0	0	0	0	0	0	0	0
24								Total	264.6	267.6	269.3	269.3	269.3	269.3	279.5	267.6
25								Uncertainty Matrix (	ocm sigma)							
26	Uncertainties(p	Pitch	Fuel Diameter	Enrichment	Fuel Length	Cluster Separation	Total	,,	LCT001-1	LCT001-2	LCT001-3	LCT001-4	LCT001-5	LCT001-6	LCT001-7	LCT001-8
27	Case1	210	100	100	70	0	264.6	LCT001-1	264.6	261.4	261.4	261.4	261.4	261.4	261.4	261.4
28	Case2	210	100	100	70	40	267.6	LCT001-2	261.4	267.6	262.1	262.1	262.1	262.1	262.7	262.0
29	Case3	210	100	100	70	50	269.3	LCT001-3	261.4	262.1	269.3	262.3	262.3	262.3	263.1	262.1
30	Case4	210	100	100	70	50	269.3	LCT001-4	261.4	262.1	262.3	269.3	262.3	262.3	263.1	262.1
31	Case5	210	100	100	70	50	269.3	LCT001-5	261.4	262.1	262.3	262.3	269.3	262.3	263.1	262.1
32	Case6	210	100	100	70	50	269.3	LCT001-6	261.4	262.1	262.3	262.3	262.3	269.3	263.1	262.1
33	Case7	210	100	100	70	90	279.5	LCT001-7	261.4	262.7	263.1	263.1	263.1	263.1	279.5	262.7
34	Case8	210	100	100	70	40	267.6	LCT001-8	261.4	262.0	262.1	262.1	262.1	262.1	262.7	267.6
36									X'							
37									1	1	1	1	1	1	1	1
38									LCT001-1	LCT001-2	LCT001-3	LCT001-4	LCT001-5	LCT001-6	LCT001-7	LCT001-8
39								LCT001-1	1.000	0.965	0.959	0.959	0.959	0.959	0.924	0.965
40								LCT001-2	0.965	1.000	0.953	0.953	0.953	0.953	0.923	0.958
41								LCT001-3	0.959	0.953	1.000	0.949	0.949	0.949	0.919	0.953
42								LCT001-4	0.959	0.953	0.949	1.000	0.949	0.949	0.919	0.953
43								LCT001-5	0.959	0.953	0.949	0.949	1.000	0.949	0.919	0.953
44								LCT001-6	0.959	0.953	0.949	0.949	0.949	1.000	0.919	0.953
45								LCT001-7	0.924	0.923	0.919	0.919	0.919	0,919	1.000	0.923
46								LCT001-8	0.965	0.958	0.953	0.953	0.953	0.953	0 923	1 000

Fig. 2. Example of the Correlation Matrix Work Sheet.

Tracing the logic, and giving users freedom to change is required because these correlation values are by necessity judgement based. The fraction of uncertainty shared between benchmark cases is related to the experimental procedure; similar experimental procedures, materials, and geometry will lead to a similar fraction of shared uncertainty. It is difficult to be too certain about uncertainty, and the amount of shared uncertainty is some value between zero and one. Reading the available information in an evaluation often provides clues that influence the judgement of the probability distribution of  $\rho_{Ai,Bi}$ . A value of zero is rarely a best estimate, nor can it be considered conservative as it causes integral experiments to be weighted too highly in an adjustment process.

If information in the evaluation does influence the judgement of the fraction of shared uncertainty in the component, then it is proposed that the best that can be done is to record the logic for assigning a certain value, and to try to assign values consistently when given the same information. If the logic is transparently recorded, then it allows for others to add additional insight, or find errors, and then revise the value without reinventing the wheel each time. The above process is encoded in decision trees.

Rules in the decision tree allow the logical choices to be stored and facilitate automated computations of the covariance by simply summing shared variance between the benchmark cases and forms the corresponding correlations matrices. We have attempted to create strawman decision trees and assign an estimate of the shared variance for leaves of the tree. It should be emphasized information in the evaluation takes precedent over the trees.

## **III. ESTIMATING COVARIANCE**

In Section XI of Reference 7, Frohner states that to construct covariance matrices one needs:

- a) An error breakdown into the various error components
- b) RMS errors for all components
- c) Enough detail about the data reduction so that sensitivity coefficients can be calculated

He also notes that the statistical errors (denoted a in Reference 7) are uncorrelated and thus don't contribute to the off diagonal terms of the covariance matrix, and that the common/shared errors (denoted b, c in Reference 7) are usually mutually uncorrelated between terms so the correlation between different terms is near zero. Section 2 the ICSBEP evaluations requires a breakdown of error into components and the uncertainty from these components which implicitly includes the magnitude of the sensitivity coefficient (but not always the sign). When error sources are fully decomposed the remaining step is to classify the uncertainty as shared or unshared between cases. When not fully decomposed one needs to either perform the

decomposition or estimate the fraction of the summed uncertainty that is shared or unshared.

## 1. Types of Uncertainties

To estimate whether the uncertainty is shared or not, it is useful to classify the uncertainties. Below are common examples that occur during ICSBEP experimental benchmarks, with some examples.

*a. The parameter has exactly the same value/realization between cases:* This leads to full correlation. Example: fuel elements that remain unchanged between cases.

b. The parameter is taken from the same distribution [i.i.d. independent with identical distributions]: This leads to a correlation between systematic errors, but no correlation between random errors. Example: fuel elements that are unloaded into a bin containing an infinite number of similar elements, with the core subsequently rebuilt by selecting from these elements. If the number of elements in the bin is close to the total number of elements shared random error is reduced.

### c. Input variable is taken from a different distribution:

Shared systematic uncertainties are correlated, some systematic uncertainties may be uncorrelated, random uncertainties are uncorrelated. Example: new fuel elements are selected, that may or may not have been enriched in the same facility.

In each case some degree of understanding of the experimental procedure is required in order to estimate the degree of correlation between the input variable uncertainties. Occasionally, decomposition of the input variable into the sources of uncertainty will be performed, and rules will be applied to the decomposed components in order to estimate the correlation between the input variables.

In summary, systematic uncertainties are often shared between cases. Random error can also be shared between cases, depending if distributions have been resampled or not. The experimenter is in the best position to elucidate the amount of resampling performed, but in the absence of such information, estimates resampling can be performed. In Section 2 of the ICSBEP Handbook, error values are most often given for the random component of the error. Any study made by the evaluator on the degree of shared uncertainty should not be overruled unless there is a good reason to do so.

Consistent with the graded approach suggest by the uncertainty guide, the estimate of the correlation coefficient will be made by considering uncertainties that contribute to 90% of the variance, which is typically the top 3 or 4 contributors. The information in the evaluation can provide relevant information when estimating if an uncertainty is shared or not.

## 2. Example Decision Trees

The process of applying consistent judgement of correlation, when given consistent information is encoded into decision trees. Some example decision trees are given for uncertainties due to pitch, see Fig. 3., and uncertainties due to the separation, see Fig. 4., between two components.



Fig. 3. Example of the Correlation Matrix Work Sheet.

Branches of the decision tree where information leads to the judgement that the same grid plate/assemblies are used. In the excel worksheet, pitch is i=2 and uncertainty from component separation is i=3, so the classification terminology will refer to rule 2 and rule 3, which are the trees for pitch and separation respectively.

Below is the decision tree for pitch, along with the judgement of the amount of shared uncertainty.

Rule 2.1: Core not rebuilt, so no elements have been resampled. Pitch uncertainty would be highly shared. [Assign  $\rho_{Ai,Bi} = 0.99$ ]

Rule 2.2: Core rebuilt, same fuel cladding, same number of elements, or elements removed. Rods would have been removed and reinstalled leading to a small difference in the uncertainty from this component; however since it is a random uncertainty divided by the root of the number of elements it is unlikely to be a large component. [Assign  $\rho_{Ai,Bi} = 0.99$ ]

Rule 2.3: Existing core with fuel elements added from the same distribution as the original elements. [Assign  $\rho_{Ai,Bi} = 0.99$ ]

Rule 2.4: New elements added to existing core, different element/cladding properties. Grid uncertainties are correlated between cases. There is less correlation due to the difference in cladding diameters. If 50% of the elements are similar between cases, then the correlation will be assumed to be at least  $\rho_{Ai,Bi} = 0.50$  (or % of similar elements). If the

experiments take place in air, or are not at all sensitive to the displacement of fluid, then the correlation will be more dependent on the grid place uncertainties and so can be taken to be  $\rho_{Ai,Bi} = 0.99$ .

[Assign  $\rho_{Ai,Bi} = \%$  of similar elements if exp is in water, and c=0.99 if exp is in air]

### New/Different Grid Plate or Assemblies used.

Rule 2.5: Fuel replaced with a different fuel type [Assign  $\rho_{Ai,Bi} = 0.0$ ]

Rule 2.6: Same fuel elements used with a different pitch/grid plate. This assumes that the uncertainty mostly dependent on the fuel and that the same manufacturing process is used for the different grids. This assumption will be refined if further information regarding the component of pitch uncertainty due to fuel vs. grid manufacture becomes available. It is based on the scenario where a pitch uncertainty has been given in the evaluation, but there is no decomposition of the uncertainty into components. [Assign  $\rho_{Ai,Bi} = 0.80$ ]

Rule 2.7: Different Fuel elements used, but sampled from the same distribution, with a different pitch/grid plate [Assign  $\rho_{Ai,Bi}$  =0.80]

So the above illustrates that the process involves reading an evaluation and deciding if one of the existing branches of the decision tree adequately describes how the experiment was done. If not, then a new branch needs to be added to the tree. Also the user can have a different assessment of the amount of shared variance from the leaves and future activities can involve comparisons of the range of judgements made by various experts.

The next example of decision trees involves the uncertainty from separation between two objects, see Fig. 4. The leaves of the tree are influenced by the experimental design. For example if the movable object is constrained to be in the same position because it is inserted into a fixed hole or groove, or whether the object freely placed between experiments. Even if two objects have moved, if they are reinserted into fixed positions, it is hypothesized that the uncertainties will be more correlated than if the positioning is arbitrary. Other leaves of tree are possible, but leaves have only been added when an experiment has been done that corresponds to a leaf. So the exercise is not to postulate all possible experimental procedures, but rather to sort the different ways an experiment has been done.



Fig. 4. Example of the Correlation Matrix Work Sheet.

Rule 3.1: Distance between two objects that haven't moved. If the source of the geometry uncertainty is not changing between cases apply a correlation of 0.99. The separation uncertainty is divided by scenarios where the object is being reinserted into a fixed position, or not. The uncertainty is further broken down if 1 or 2 objects are being moved. The logic is that in general if an object is being continually reinserted into fixed positions, the uncertainty from the position will be more correlated between cases then if the objects are not being put into fixed positions as the later scenario will have more random uncertainty. [Assign  $\rho_{Ai,Bi} = 0.99$ ]

### Moving objects not fixed:

Rule 3.2: Distance between a stationary object and movable object. In this case the position of one object has changed. The uncertainty associated with the measuring equipment is likely the same, so the systematic component of the measurement uncertainty will result in correlation between the cases, while the random component will be uncorrelated. [Assign  $\rho_{Ai,Bi} = 0.5$ ]

Rule 3.3: Distance between two moveable objects. In this case the position of both objects have changed. The uncertainty associated with the measuring equipment is likely the same, so the systematic component of the measurement uncertainty will result in correlation between the cases, while the random component will be uncorrelated. Moving objects, being reinserted into fixed/constrained positions. [Assign  $\rho_{Ai,Bi} = 0.2$ ]

Rule 3.4: Distance between a stationary object and movable object. [Assign  $\rho_{Ai,Bi} = 0.9$ ]

Rule 3.5: Distance between two moveable objects. [Assign  $\rho_{Ai,Bi} = 0.7$ ]

The trees allow expedite the process of judgement, as if the procedure fits in a certain logical bin the user can rapidly look up an estimate of what correlation coefficient could be assigned. Furthermore, if they have a different judgment that correspond to the leaf of the tree, it is easy to overwrite the values in the excel sheet.

### **IV. TESTING COVARIANCE**

Nuclear data covariance matrices are constructed based on the best possible estimates of the true covariance, and so are not linked to a particular application. In the same way, covariance's between integral experimental benchmarks should be application independent. In this section, general results are shown that provide an estimate of the impact adding experimental covariance to a generalized least squares code which is attempting to provide best estimates of parameters given both nuclear data and experimental data best estimate values and uncertainties.

Using the TSURFER routine in SCALE6.2 the impact of an experimental covariance matrix was analyzed. The tests were simplistic studies running the code with and without experimental correlations. The input data for all the runs consisted of sensitivity profiles computed using the 238 group ENDF/B-VII.0 library distributed with SCALE and the 44 energy group nuclear data covariance library. The C/E values were done with continuous energy KENO using the ENDF/B-VII.0 library as these calculated results had a lower uncertainty from modelling approximations. Results presented in the following sections comprise the standard available output from a TSURFER calculation.

## 1. Chi Squared Test

As far as the authors know, there is no foolproof test of the adequacy of an experimental covariance matrix. It is possible that better known and unknown tests exist.

Chi squared per degrees of freedom is a commonly used test that provides information on the consistency of the C-E discrepancies with the given uncertainty matrices. High chi squared values can mean that the nuclear data, or experimental uncertainties have been underestimated, or the correlation terms have been underestimated. Also undetected errors and biases will tend to increase chi squared. So when applying the metric it should be kept in mind that the existing combined nuclear data and experimental uncertainty matrix is being assessed.

The results of the chi squared test were analyzed. In TSURFER Chi squared values are computed using the initial discrepancy vector [C-E] **di** and the inverse of the full covariance matrix, **Vij**, which includes nuclear data and experimental covariance.

$$\chi^2 = \sum_i \sum_j d_i V_{i,j}^{-1} d_j \tag{Eq. 3}$$

Two cases were examined, the initial chi squared values with and without covariance. Chi squared values were examined within an evaluation, so the plot shows chi

squared values for each evaluation were correlations were derived see Fig. 5. Note that increasing the degree of correlation has the effect of reducing the number of degrees of freedom. In the limit of full correlation, performing many experiments is the same as performing a single experiment, conversely, uncorrelated results are independent and thus represent the maximum number of degrees of freedom. This means that adding correlation data to an analysis while increase the initial chi squared per degrees of freedom value.



Fig. 5. Example of the Correlation Matrix Work Sheet.

The initial chi squared values per degree of freedom for uncorrelated results usually below one, while when using correlation the value is typically above one. Clearly the assignment of correlation values changes the perception of whether the total, both nuclear data and experimental uncertainties are underestimated or not. Since removing an experiment should be done with caution and for justified reasons, no chi squared filter was applied here; however it is clear that some experimental values would be need to be further scrutinized if the correlated values are considered reasonable.

# 2. Standard Deviation Test

The chi squared metric is sensitivity to biases, rather than the spread, so the next test was simply to examine the spread of C-E values after a generalized least squares fit both with and without experimental correlations as shown in Fig. 6. This test is more sensitive to C-E values that deviate from the average C-E value in a series; the metric is a measure of the random error within a series. If the experiments are uncorrelated the spread should be at least the experimental benchmark uncertainty. Additional spread would occur from the uncorrelated part of the nuclear data uncertainties.

The figure shows that the spread in C-E is often less than the experimental benchmark uncertainty, the grey shading, which is strongly consistent with there being correlations; the graph does not rule out the possibility of experimental uncertainties being overestimated in some cases.



Fig. 6. Comparison of calculated C-E standard deviation, with the experimental uncertainty.

#### 3. Nuclear Data Adjustment Test

The final test examined the proposed nuclear data cross section adjustments both with and without experimental benchmark correlations. Adjustments were performed both within an experimental series and for the full set of cases where all benchmarks where placed into a single TSURFER input. Fig. 7. Shows the results for U<sup>238</sup> inelastic and elastic cross section in the fast energy region, which was chosen as it had amongst the largest adjustments for each evaluation series. It is informative to compare the proposed LCT com adjustment with and without correlations. The result is significantly different, as the uncorrelated adjustments are large as they are of the order of 40%, while the correlated adjustments are quite small and in the same direction. It is also interesting to see that the purposed adjustment for the full case is larger than the adjustments of any of the individual cases. When performing adjustments it should be kept in mind that we are working with a highly underdetermined system, and so the statistical power of the individual cases is quite low, but it appears that for the correlated cases a fairly stable proposed adjustment is proposed.

### V. CONCLUSIONS

A database of uncertainties from ICSBEP evaluations has been created and used to create covariance matrices for cases within an evaluation. The covariance matrices are constructed based upon the judgement of the amount of shared uncertainty between cases. The results of testing the impact of the generated covariance matrices on standard metrics such as chi-squared, comparison of residuals, and nuclear data adjustment supported that the experimental benchmark uncertainties are correlated. Results were strongly influenced by the inclusion of covariance matrices. Further testing on specific applications is warranted.

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Fig. 7. Fast cross section adjustments to U<sup>238</sup> inelastic and elastic scattering cross section during TSURFER nuclear data adjustment, with and without correlations.