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APPENDICES

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1. Introduction

A method using MCNP6 with sensitivity and uncertainty data to determine the baseline Upper Subcritical Limits is discussed in:

- LA-UR-14-26558, *Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits*
- LA-UR-14-23202, *Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation*
- LA-UR-14-23352, *Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems*

The Whisper Fortran program (Version 1.0.0) and various script files were developed to implement the methodology described in these three documents (although LA-UR-14-23202 and LA-UR-14-23352 do not reference Whisper by name). In this report, the Whisper Fortran program and script files are collectively called the Whisper program suite. The user instructions for the Whisper program suite are given in:

- LA-UR-14-26436, *User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation*

However, none of these documents explain the internal operation of the Whisper Fortran program or the script files. An inspection review of the Whisper Fortran source code was performed in the *Whisper Source Code Inspection Report*. Therefore, the internal operation of the Whisper Fortran code is not covered in this report, although the source code inspection is credited for its verification and validation (V&V) value. To provide V&V of the Whisper program suite, this report reviews the script files. This report is organized by the functions performed by the Whisper program suite. The report starts with the most common function that criticality safety analysts will perform: evaluation of an application model and calculation of the corresponding baseline USL. Generally, the sections include descriptions of:

1. the output data,
2. the input data,
3. the algorithm (i.e., what needs to be done),
4. the process (i.e., the user actions and computer programs), and
5. the computer programs.

For each computer program (e.g., script file), the generic command syntax, operations, V&V (verification and validation) activities, and V&V results are discussed.

1.1 Executable Programs

The Whisper program suite consists of the following executable files (in order of appearance):

1. Whisper/bin/whisper (executable from Fortran source code)¹
2. Whisper/bin/whimcnp (csh script file)
3. Whisper/Utilities/RunMCNPInputs.csh
4. Whisper/bin/ww (csh script file)
5. Whisper/Utilities/MakeKeffSenLib.csh
6. Whisper/Utilities/CovarianceData/ProcessCovData.csh
7. Whisper/Utilities/CovarianceData/CopyUnadjustedData.csh
8. Whisper/Utilities/Benchmarks/AppendBenchmarks.csh
9. Whisper/Utilities/CovarianceData/UpdateCovariance.csh
10. Whisper/Utilities/Testing/UpdateInstallSolutions.csh
11. Whisper/Testing/Makefile (a GNU Make utility command file)
12. Whisper/Testing/Installation/RunInstallTests.csh
13. Whisper/Install/InstallWhisper.csh
14. Whisper/Install/UninstallWhisper.csh
15. Whisper/Makefile
16. Whisper/Source/Makefile

1.2 Scope

This report examines each of the following functions in detail:

1. Evaluate Application Model and Calculate Baseline USL
2. Evaluate Benchmark Cases
3. Use Benchmark Experimental Correlation Data
4. Reject Inconsistent Benchmark Cases
5. Process Covariance Data
6. Append New Benchmark Cases
7. Create New Covariance Directory and Data
8. Replace Default Covariance Data
9. Updating Installation Test Reference Solutions
10. Run Installation Tests

This report does not include a review of the benchmark models which generated the sensitivity coefficients used by Whisper.

¹ Originally compiled in directory Whisper/Source/whisper.

2. Conclusions

During the preparation of this report, the following issues were identified:

1. The correlation data file (Benchmark/Correlations/BenchCorrel.dat) has two discrepancies with the correlation matrix (September 2013 Edition of DICE). XCP-3 reported that the significance and impact of these two errors should be negligible because the correlation data is used only in the rejection of benchmarks. Other than the rejection process to exclude benchmarks from further consideration, the correlation data is not used in calculating the calculational margin value. The four benchmarks involved in these two errors were not rejected; therefore, the incorrect correlation data did not result in any erroneous benchmark rejections. See Section 5 below for additional information.
2. Whisper V1.0.0 is not using the correct covariance data for the meta-stable isotopes because the ORNL covariance data and MCNP6 cross section library use different identifiers. However, none of the benchmark models distributed with Whisper V1.0.0 include any of the listed isotopes. Therefore, the fact that the covariance data for these isotopes is missing or incorrect does not affect the final results for any application model. See Section 7.5.1 and Appendix G for more information.

In addition to the V&V activities documented in this report, an inspection of the Fortran source code for Whisper V1.0.0 was documented in the *Whisper Source Code Inspection Report*.

3. Evaluate Application Model and Calculate Baseline USL

The most common Whisper program suite function that criticality safety analysts will perform is the evaluation of an application model and calculation of the corresponding baseline USL. For example, for validation report LA-UR-14-23352, application models were prepared for plutonium metals, solutions, and oxides; and different reflector materials and thicknesses around plutonium metal. These application models were evaluated and USLs calculated.

3.1 Output Data

This process creates a Whisper output file that reports the baseline USL value for the application model. The Whisper program result is a baseline USL because Whisper considers only the critical experiment benchmarks, transport software, and nuclear data, which are only a part of the overall analysis that goes into a criticality safety evaluation [LA-UR-14-26558; Sec. II]. The baseline USL should be viewed as an upper bound for the actual USL applied in a criticality safety evaluation. The baseline USL is a guide to help the analyst, and the analyst may need to apply additional margin where the baseline is, based upon expert engineering judgment, insufficient [LA-UR-14-26558; Sec. III].

3.2 Input Data

To evaluate an application model, the following data is required.

1. An MCNP6 model of the application is required. The MCNP6 input file is developed by the user.

2. This section assumes the k_{eff} sensitivity data for the benchmark cases and covariance data is available. This data is distributed with the Whisper program suite or the user can create their own data. The development of the sensitivity and covariance input data is explained in Sections 4 and 7.
3. If certain benchmark cases are to be excluded from the evaluation, the rejected benchmark data must also be available. The development of the rejection input data is explained in Section 5.4.
4. The energy grid data file (SCALE44ErgGrid.dat) distributed with the Whisper program suite is also required for input.
5. The following table [LA-UR-14-26436; Table II] lists all of the Whisper program input parameters, most of which are used when calculating the baseline USL. If a user is executing Whisper on a command line, they can replace the default value; see LA-UR-14-26436, Section 6.1. However, the script files ww and MakeKeffSenLib.csh (described below) only use the Whisper default values. In the following process flowcharts, these input parameters will not be shown as input to the Whisper program.

Whisper Parameter	Default	Description
ThresholdChiSquare	1.2	Threshold of acceptable GLLS nuclear data adjustment χ^2 for benchmark rejection.
CalcMarginConfidenceLevel	0.99	Value of the extreme value cumulative distribution function (CDF) that is used to determine the calculational margin.
dxCalcMargin	1.e-5	When determining the calculational margin from the extreme value CDF, the candidate calculational margin is increased by this amount until it is found.
dxAcceptSimilarity	1.e-5	Value that the factor to determine acceptance similarity parameter decreases by until the minimum benchmark weight is met and weight factors are determined.
MinimumWeightSum	25	The minimum total benchmark weight allowed when determining the calculational margin.
WeightSumPenalty	100	The penalty applied to the amount of benchmark weight needed for determining the calculational margin based upon the maximum similarity parameter of the benchmark set.

Whisper Parameter	Default	Description
MinimumNonCoveragePenalty	0.05	The lowest allowed non-coverage penalty applied based upon the degree of inadequacy of the entire benchmark set to meet the minimum benchmark weight.
DataUncMultiplier	2.6	Confidence level, in number of standard deviations, multiplied by the nuclear data uncertainty to get the nuclear data driven margin of subcriticality.
UnknownDataUncertainty	0.1	Value of the uncertainty along the diagonal used for covariance data that is needed but unavailable.
AdjustedCovarianceCutoff	1.e-6	Lowest value of diagonal variance that is for writing a block to the adjusted covariance data file.
IntegrationTolerance	1.e-9	Integration tolerance for residual when computing the bias from mean of the extreme value density function.
IntegrationLimitTolerance	1.e-6	Tolerance for limits of integration when computing the bias from mean of the extreme value density function.

3.3 Algorithm Description

For the Whisper program suite, evaluating application models and calculating the corresponding baseline USL is a two-step process:

1. Determine the sensitivity coefficients ($S_{k,x}$) for the application model.
 - a. The definition of sensitivity coefficient is [LA-UR-14-26558; eq. 28]:

$$S_{k,x} \equiv \frac{x}{k} \frac{\partial k}{\partial x}$$
 - b. The nuclear reactions considered are elastic scattering, inelastic scattering, fission, capture [(n,2n), (n, γ), (n,p), (n,d), (n,t), (n, 3 He), (n, α)], fission total v, and fission χ [LA-UR-14-23352; Sec. 3.1] [LA-UR-14-26436; Sec. 3.4]. All other reactions are going to be minor to criticality safety and are ignored [LA-UR-14-26436; Sec. 3.4].
 - c. Sensitivity coefficients are also specific to (binned by) the neutron energy and the isotope.

2. Use the Whisper Fortran program to calculate the calculational margin and the margin of subcriticality for the nuclear data. Whisper uses these results, and a predefined margin of subcriticality for the software, to calculate the baseline Upper Subcritical Limit:

$$\text{USL}_{\text{baseline}} = 1.0 - \text{CM} - \text{MOS}_{\text{data}} - \text{MOS}_{\text{software}}$$

The *Whisper Source Code Inspection Report* explains the Whisper Fortran program, e.g., algorithms and program operations, in detail.

3.4 Process Description

The algorithm for evaluating the application models and calculating the USLs has been implemented in MCNP6 and the Whisper program suite. The Whisper program suite includes script files further simplify the process. This section explains the method for evaluating the application models and calculating the USLs using the script files. The execution and data flow for this process is shown in Figure 3-1.

In the process flow charts, the computer programs are represented by black boxes and text. The program input arguments shown in square brackets [] are optional. The black arrows indicate that a program automatically initiates the execution of the next program. If necessary, the computer programs are numbered to illustrate the execution order. The red blocks, text, and arrows represent the user input files for this process. Other data files have blue blocks, text, and arrows.

Algorithm Step 1 in Section 3.3 above (determine the sensitivity coefficients for the application models) is performed with MCNP6. MCNP6 uses the Iterated Fission Probability (IFP) method to compute the sensitivity coefficients in a continuous-energy Monte Carlo simulation [LA-UR-14-23202; Sec. 2]. The energy grid matches the 44-group covariance library from ORNL. The second algorithm step is performed with the Whisper program. The *Whisper Source Code Inspection Report* explains the Whisper Fortran program in detail.

The USLs can be calculated without the script files but the user must manually perform many of the functions programmed into the script files.

3.4.1 MCNP6 Input Files

In order to evaluate the application models and calculate the USLs, the user must prepare MCNP6 input files for the application models. The MCNP6 input files must follow the following rules [LA-UR-14-26436; Sec. 2.3]:

1. The input file must contain the kcode card.
2. The input file may not contain prdmp, kopts, or ksen cards.

It is preferable that the application models input file not have the benchmark k and uncertainty comment (see Section 4.4.1 below for the explanation of the benchmark k and uncertainty comment). However, if the comment is included in the application model file, the values are ignored. [LA-UR-14-26436; Sec. 3.1]

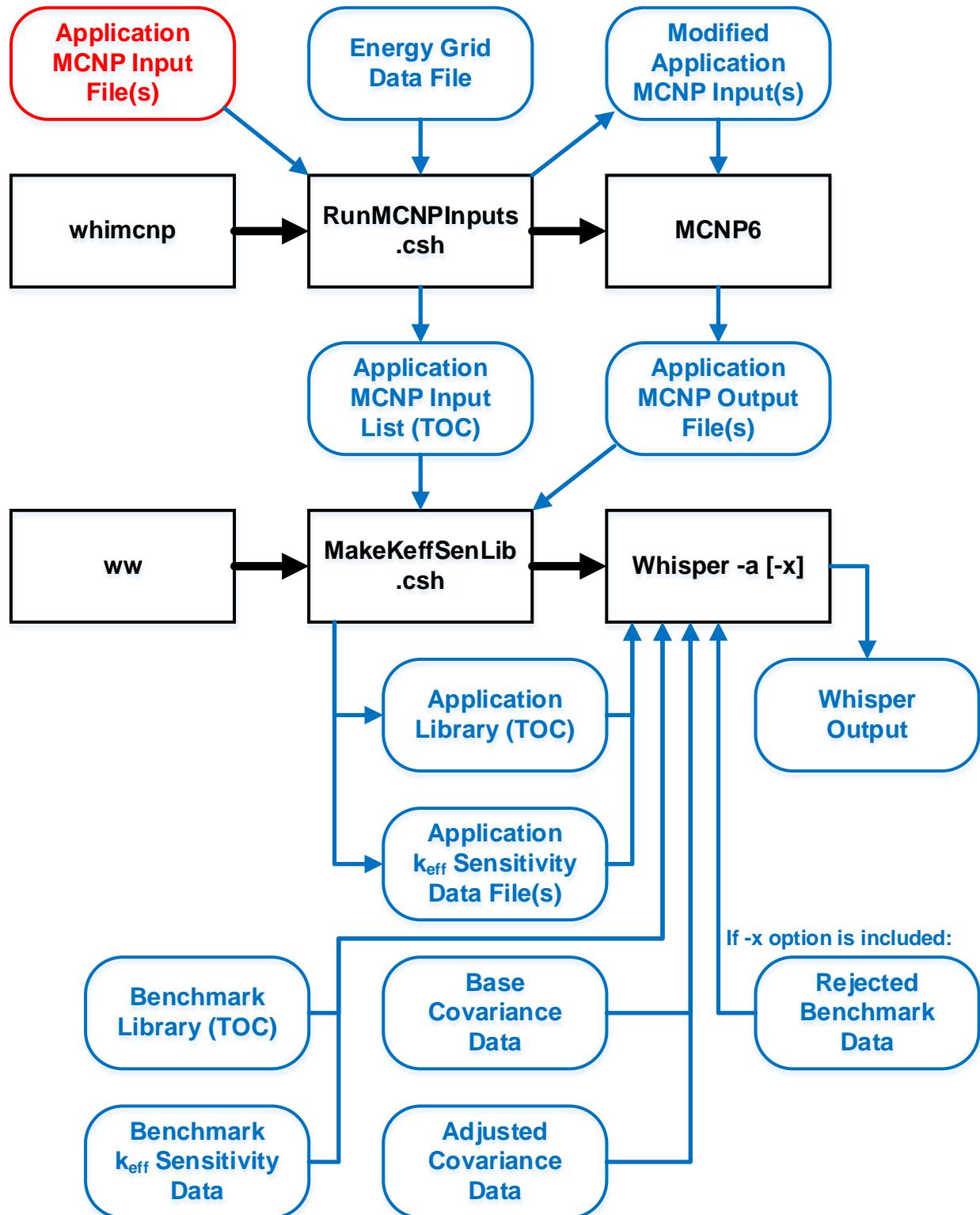


Figure 3-1
Application Model Evaluation Flowchart

3.4.2 Command Lines

To evaluate the application models, the user needs to execute the whimcnp script in the directory where the application model input files are located. As shown in Figure 3-1, whimcnp will invoke RunMCNPInputs.csh, which then runs MCNP6. The command syntax is² [LA-UR-14-26436; Sec. 2.3]:

```
> whimcnp [walltime hh:mm:ss] inp1 [inp2] ...
```

When all of the MCNP6 runs are completed³, the Whisper wrapper (ww) program is executed. As shown in Figure 3-1, ww will invoke MakeKeffSenLib.csh, which will run Whisper. To execute ww, the command syntax is [LA-UR-14-26436; Sec. 3.2]:

```
> ww [ExcludeFile.dat]
```

When executing ww on a multi-node platform, such as Moonlight, the user may need to login to a compute node (with the llogin command) before executing ww.

The script files whimcnp and ww are explained below.

3.5 Computer Programs

3.5.1 Script File whimcnp

3.5.1.1 Command Syntax

As given above, the syntax to execute whimcnp is:

```
> whimcnp [walltime hh:mm:ss] inp1 [inp2] ...
```

where

walltime hh:mm:ss	= changes the wall-clock submission time from the default of one hour (optional).
inp1	= the name of the first MCNP6 input file (required).
inp2	= the name of the second MCNP6 input file (optional). Additional MCNP6 input files can be specified as desired.

² The computer prompt for a command line is shown as “>”. Any lines not beginning with the command prompt are continuations of the previous line.

³ This condition can be satisfied by either (1) the user waiting until all jobs initiated by whimcnp have finished before proceeding [LA-UR-14-26436; Sec. 3.1], or (2) submitting the ww job with dependencies. For submitting with dependencies, the reader should research the depend parameter on the ms sub command.

The whimcnp script works with the wildcard character “*” in the filename(s). For example, to execute the whimcnp script with all files in the current directory with the extension “inp” (with the default time limit of one hour), use the command:

```
> whimcnp *.inp
```

3.5.1.2 Operations

Script file whimcnp performs the following:

1. Checks whether the file ‘MCNPInputList.toc’ exists. If the file ‘MCNPInputList.toc’ does exist, whimcnp exits with an error message, to prevent accidentally overwriting ‘MCNPInputList.toc’ [LA-UR-14-26436; Sec. 3.1].
2. Checks whether lowest directory in the WHISPER_PATH environment variable is ‘Whisper’. If not, whimcnp exits with an error message.
3. Checks whether one or more arguments are provided to whimcnp. If not, whimcnp exits with an error message.
4. Executes the script file RunMCNPInputs.csh as follows [LA-UR-14-26436; Sec. 3.1]:

```
> $WhisperDir/Utilities/RunMCNPInputs.csh [walltime  
hh:mm:ss] MCNPInputList.toc inp1 [inp2] ...
```

The optional arguments ‘walltime hh:mm:ss’ are included only if the user specified them on the whimcnp command line.

3.5.1.3 V&V Activities

Script file whimcnp can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers⁴.

Operation Step	Script line numbers
1.	7 – 12
2.	14 – 18
3.	20 – 24
4.	26 – 31

⁴ The algorithm section summarizes the primary logic and calculations for the script file. The script file contains statements that, although essential for program operation, do not directly correspond to an algorithm step. Examples include variable assignments, logic branches corresponding to error conditions, etc. It is presumed that a reader familiar with Linux and C shell or GNU Make (depending on the script file) will understand the statements not discussed in the summary.

3.5.1.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

3.5.2 Script File RunMCNPInputs.csh

3.5.2.1 Command Syntax

The general syntax for script file RunMCNPInputs.csh is [LA-UR-14-26436; Sec. 3.1]:

```
> RunMCNPInputs.csh [walltime hh:mm:ss] MCNPInput.toc inp1  
[inp2] ...
```

where

- walltime *hh:mm:ss* = changes the wall-clock submission time from the default of one hour (optional).
- MCNPInput.toc* = output file listing the MCNP6 input files and any benchmark *k* values and uncertainties that are provided in the MCNP6 input files.
- inp1* = the name of the first MCNP6 input file (required).
- inp2* = the name of the second MCNP6 input file (optional). Additional MCNP6 input files can be specified as desired.

Note: Script RunMCNPInputs.csh will overwrite the file *MCNPInput.toc* [LA-UR-14-26436; Sec. 3.1].

3.5.2.2 Operations

Script file RunMCNPInputs.csh performs the following:

1. Checks that the file ‘SCALE44ErgGrid.dat’ exists, either locally (take precedence) or under the WHISPER_PATH directory (e.g., in the subdirectory /Utilities/Data)
2. Creates the MCNP6 input list (table of contents) file; with script file whimcnp, the filename is always MCNPInputList.toc. For each input file on the command line, a record is written to the MCNP6 input table of contents file. The record format is:
 - a. MCNP6 input filename (without the directory path)
 - b. Benchmark k_{eff} – from the comment in the MCNP6 input file (see Sec. 4.4.1 below)
 - c. Benchmark uncertainty – from the comment in the MCNP6 input file (see Sec. 4.4.1)

3. Creates the subdirectory ‘Calcs’ (if it does not exist).
4. Creates the subdirectory ‘KeffSenLib’ (if it does not exist).
5. For each given MCNP6 input file, if the sensitivity file does not exist in the ‘KeffSenLib’ directory:
 - a. Creates a modified MCNP6 input file in the Calcs directory,
 - 1) Copies the given file up to (but not including) the kcode line.
 - 2) Writes the following MCNP6 input lines:

```
kcode 100000 1.0 100 600
kopts blocksize = 5
ksen1 xs
```
 - 3) Writes the energy grid to the MCNP6 input file.
 - a) The energy grid is obtained from a file called SCALE44ErgGrid.dat, which must be available either locally (takes precedence) or in the directory Whisper/Utilities/Data [LA-UR-14-26436; Sec. 3.1].
 - b) The ‘SCALE44ErgGrid.dat’ file distributed with Whisper is:

```
rxn = +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
erg = 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
      4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
      2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
      4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
      6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
      3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
      1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
      6.4340e+00 8.1873e+00 2.0000e+01
```

- 4) Writes the following MCNP6 input line:


```
prdmpr    j    9999999
```
- 5) Copies the given file after the kcode line.
- b. Deletes the corresponding MCNP6 output (o suffix), run tape (r suffix), and source tape (s suffix) files in directory Calcs.
- c. Creates a job file.
- d. Submits the job file for execution.
- e. Deletes the job file.

3.5.2.3 V&V Activities

Script file RunMCNPInputs.csh can be verified and validated by:

1. a review of the script file,
2. verifying the contents of the MCNPInputList.toc file, and
3. verifying the modified MCNP6 input files.

3.5.2.3.1 Script File Review

The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	35 – 45
2.	82 – 95
3.	99 – 101
4.	102 – 104
5.	108 – 173
5.a.1	120 – 125
5.a.2	126 – 128
5.a.3	129
5.a.4	130
5.a.5	132 – 135
5.b	140 – 155
5.c	157 – 161
5.d	164
5.e	165

3.5.2.3.2 MCNPInputList.toc File

The contents of the MCNPInputList.toc file in the Moonlight directory Whisper/ValidationFiles/vv/pumetal are (after the line numbers):

1	pumetal_0.01_in	0.0000	0.0000
2	pumetal_0.02_in	0.0000	0.0000
3	pumetal_0.03_in	0.0000	0.0000
4	pumetal_0.04_in	0.0000	0.0000
5	pumetal_0.05_in	0.0000	0.0000
6	pumetal_0.06_in	0.0000	0.0000
7	pumetal_0.07_in	0.0000	0.0000

8	pumetal_0.08_in	0.0000	0.0000
9	pumetal_0.09_in	0.0000	0.0000
10	pumetal_0.11_in	0.0000	0.0000
11	pumetal_0.12_in	0.0000	0.0000
12	pumetal_0.13_in	0.0000	0.0000
13	pumetal_0.14_in	0.0000	0.0000
14	pumetal_0.15_in	0.0000	0.0000
15	pumetal_0.16_in	0.0000	0.0000
16	pumetal_0.17_in	0.0000	0.0000
17	pumetal_0.18_in	0.0000	0.0000
18	pumetal_0.19_in	0.0000	0.0000
19	pumetal_0.1_in	0.0000	0.0000
20	pumetal_0.2_in	0.0000	0.0000
21	pumetal_1e-06_in	0.0000	0.0000

Although the whimcnp and RunMCNPInputs.csh commands are not available for comparison, The filenames match the MCNP6 input files in the directory. The benchmark k_{eff} and uncertainty defaulted to zero because the MCNP6 input files do not have the comment with these values; an example input file is provided in Appendix A.

3.5.2.3.3 Modified MCNP6 Input Files

Appendix A compares an original MCNP6 input file with the modified file produced by RunMCNPInputs.csh. The file modifications match Operation step 5.a above.

3.5.2.4 V&V Results

The results of the V&V activities are:

1. The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.
2. The contents of a MCNPInputList.toc file used in the validation on the Moonlight platform:
 - a. Corresponds to the format in Operation step 2 above.
 - b. The filenames match the MCNP6 input files in the directory.
3. The MCNP6 input file modifications performed by RunMCNPInputs.csh correspond to Operation step 5.a above.

3.5.3 Script File ww

3.5.3.1 Command Syntax

As given above, the syntax to execute ww is [LA-UR-14-26436; Sec. 3.2]:

```
> ww [ExcludeFile.dat]
```

where

ExcludeFile.dat = file containing a list of benchmarks (one per line) to be excluded from the validation (optional).

It is useful to leave out irrelevant benchmarks for the validation, e.g., exclude uranium systems for a plutonium validation, to save time [LA-UR-14-26436; Sec. 3.2].

3.5.3.2 Operations

Script file ww performs the following:

1. Checks whether lowest directory in the WHISPER_PATH environment variable is ‘Whisper’. If not, ww exits with an error message.
2. Checks whether file MCNPInputList.toc exists. If MCNPInputList.toc does not exist, ww exits with an error message.
3. If an *ExcludeFile.dat* file is specified but the file does not exist, ww exits with an error message.
4. Executes the script file MakeKeffSenLib.csh as follows [LA-UR-14-26436; Sec. 3.2]:

```
> $WhisperDir/Utilities/MakeKeffSenLib.csh  
MCNPInputList.toc KeffSenList.toc run [ExcludeFile.dat]
```

The optional argument *ExcludeFile.dat* is included only if the user specified the filename on the ww command line.

3.5.3.3 V&V Activities

Script file ww can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	11 – 14
2.	16 – 19
3.	22 – 26
4.	27 or 29

3.5.3.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

3.5.4 Script File MakeKeffSenLib.csh

3.5.4.1 Command Syntax

The syntax for script file MakeKeffSenLib.csh is:

```
> MakeKeffSenLib.csh MCNPInput.toc KeffLib.toc [run]  
[ExcludeFile.dat]
```

where

<i>MCNPInput.toc</i>	= input file listing the MCNP6 input files and any benchmark k_{eff} values and uncertainties that are provided in the MCNP6 input files (required).
<i>KeffLib.toc</i>	= name of the sensitivity library that will be used by Whisper.
<i>run</i>	= keyword argument to have the script run Whisper (optional) [LA-UR-14-26436; Sec. 3.2].
<i>ExcludeFile.dat</i>	= file containing a list of benchmarks (one per line) to be excluded from the validation (optional). It is useful to leave out irrelevant benchmarks for the validation, e.g., exclude uranium systems for a plutonium validation, to save time. [LA-UR-14-26436; Sec. 3.2]

When MakeKeffSenLib.csh is invoked by the script file ww, (1) the KeffLib.toc filename is always KeffSenList.toc and (2) run is always specified.

3.5.4.2 Operations

Script file MakeKeffSenLib.csh performs the following:

1. Checks whether the MCNPInput.toc file exists. If the MCNPInput.toc file does not exist, MakeKeffSenLib.csh exits with an error message.
2. Checks whether the subdirectory Calcs exists. If subdirectory Calcs does not exist, MakeKeffSenLib.csh exits with an error message.
3. Checks whether the subdirectory KeffSenLib exists. If subdirectory KeffSenLib does not exist, MakeKeffSenLib.csh exits with an error message.
4. Creates the KeffLib.toc file.
 - a. If the KeffLib.toc file exists, MakeKeffSenLib.csh replaces the file.

- b. The full pathname to directory KeffSenLib is the first line written to the KeffLib.toc file.
5. For each record in the MCNPInput.toc file:
 - a. The sensitivity data is extracted from the output file (in the Calcs directory) and written to the corresponding sensitivity (suffix k) file in the KeffSenLib directory.
 - 1) The sensitivity data begins on the second line after the text string “sensitivity profile” and ends two lines before the test string “1average”.
 - b. Write the k_{eff} sensitivity data to the KeffLib.toc file (e.g., KeffSenList.toc). Each line of the file contains [LA-UR-14-26436; Sec. 3.4]
 - 1) MCNP6 input filename (without the directory path)
 - 2) Benchmark k_{eff} – from the MCNPInput.toc file
 - a) For an application, this is normally zero and a non-zero value will be ignored by the Whisper program.
 - 3) Benchmark uncertainty – from the MCNPInput.toc file
 - a) For an application, this is normally zero and a non-zero value will be ignored by the Whisper program.
 - 4) Application model k_{eff} – from the MCNP6 output file; on the line with the test string “final estimated”
 - 5) Application model uncertainty – from the MCNP6 output file; on the line with the test string “final estimated”

6. If the “run” argument is specified, execute the whisper code as follows:

```
> whisper -a KeffLib.toc [-x ExcludeFile.dat]
```

The optional argument “-x *ExcludeFile.dat*” is included only if the user specified an exclude filename on the MakeKeffSenLib.csh (or ww) command line.

3.5.4.3 V&V Activities

Script file MakeKeffSenLib.csh can be verified and validated by:

1. a review of the script file,
2. verifying the contents of the KeffSenList.toc

3.5.4.3.1 Script File Review

The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	38 – 41
2.	42 – 45
3.	46 – 49
4.a	52 – 54
4.b	55
5.	57 – 105
5.a	61 – 88
5.b	90 – 96
6.	111 – 127

3.5.4.3.2 KeffSenList.toc Contents

The contents of the KeffSenList.toc file in the Moonlight directory Whisper/ValidationFiles/vv/pumetal are listed in Appendix B. The format corresponds to Operation step 5.b above. The application k_{eff} and uncertainty values in the KeffSenList.toc file match the MCNP6 results.

3.5.4.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

The format of the KeffSenList.toc file corresponds to Operation step 5.b above. The application k_{eff} and uncertainty values in the KeffSenList.toc file match the MCNP6 results.

3.5 Whisper Program

3.5.5.1 Command Syntax

The Whisper code has several possible command line arguments; see Table I of LA-UR-14-26436 for the full list. The script file MakeKeffSenLib.csh executes Whisper with the command:

```
> whisper -a KeffSenList.toc [-x ExcludeFile.dat]
```

The optional arguments “-x *ExcludeFile.dat*” is included only if the user specified an exclude filename on the MakeKeffSenLib.csh (or ww) command line.

3.5.5.2 Operations

The Whisper code performs algorithm steps 2 through 6 in Section 3.3 above.

3.5.5.3 V&V Activities

The V&V activities for the Whisper code are:

1. Verify the energy grid matches the 44-group covariance library from ORNL.
2. The reaction numbers in the MCNP6 input files must correspond to the relevant MTs in the Whisper code.
3. Compare the calculational margins calculated by Whisper against the calculational margin results from traditional methods.
4. Review the Whisper source code.

3.5.5.3.1 Energy Grid Verification

Appendix C compares the energy grid in the ‘SCALE44ErgGrid.dat’ file distributed with Whisper against the energy bins in the ORNL covariance data file (Whisper/CovarianceData/SCALE6.1/Native/ORNL_SCALE6.1.cov). After accounting for differences in units and ordering, the two sets of energy boundaries are identical.

3.5.5.3.2 Reaction Number Verification

Appendix D compared the reaction numbers in the ‘SCALE44ErgGrid.dat’ file distributed with Whisper against the relevant MTs programmed into the Whisper code. Although there are apparent differences between some values, the reaction numbers and relevant MT values correspond to the same reaction data.

3.5.5.3.3 Comparisons Against Traditional Methods

LA-UR-14-26558 includes a suite of test problems that verify the correct installation of the Whisper program. LA-UR-14-26558 Table IV compares the Whisper calculational margin results for five cases against the results from the traditional parametric method and the non-parametric, rank-order method.

Compared to the parametric method, which requires benchmark data to be normally distributed, Whisper typically obtains similar or more conservative calculational margins [LA-UR-14-26558; Abstract]. Because Whisper uses an extreme value distribution, Whisper is expected to be more conservative than the parametric method, which uses a weighted average [LA-UR-14-26558; Sec. V.E]. The exception to this expectation can occur when Whisper identifies and uses benchmark models that are neutronically similar to the application case, which are not used in the traditional parametric method because the material forms are dissimilar, i.e., oxide vs. metal or solution [LA-UR-14-26558; Sec. V.E].

Compared to the non-parametric, rank-order method, Whisper obtains less stringent calculational margins [LA-UR-14-26558; Abstract]. Whisper results are expected to be less stringent than the non-parametric, rank-order method because Whisper uses neutronic similarity weighting whereas the rank-order method simply uses the worst case [LA-UR-14-26558; Sec. V.E].

3.5.5.3.4 Whisper Source Code Inspection

A thorough inspection of the Whisper source code was performed. The *Whisper Source Code Inspection Report* explains how and where the LA-UR-14-26558 equations and algorithms were implemented in the Whisper source code.

3.5.5.4 V&V Results

The results of the V&V activities for the Whisper code are:

1. The energy grid in the ‘SCALE44ErgGrid.dat’ file distributed with Whisper matches the 44-group covariance library from ORNL.
2. The reaction numbers in the MCNP6 input files correspond to the relevant MTs in the Whisper code.
3. The calculational margins from Whisper and the traditional methods are similar enough to indicate Whisper produces reasonable calculational margins. Exactly identical results from the different methods were not expected.
4. The review of the Whisper source code was performed in the *Whisper Source Code Inspection Report*.

4. Evaluate Benchmark Cases

The previous section assumed the k_{eff} sensitivity data for the benchmark cases was available for use. If the benchmark data is distributed with the Whisper program suite is sufficient and appropriate, this is a valid assumption. This section explains how the k_{eff} sensitivity data for the benchmark cases was created. Users can use this process to create their own benchmark k_{eff} sensitivity data. However, if the user desires to append additional new benchmark cases to the current benchmarks, rather than replacing the current benchmarks, see Section 8 below.

The benchmark cases distributed with the Whisper program suite were either developed during previous validation efforts, or prepared (and independently reviewed) for the Whisper benchmark suite. The previous validations used are [LA-UR-14-26558; Sec. IV.B] [LA-UR-14-23352; Sec. 3]:

1. Previous NCS validation suite [NCS-TECH-007-002]
2. Mosteller Expanded Criticality Suite for MCNP6 validation [LA-UR-10-06230, Rev 3]
3. Kahler validation suite for ENDF/B-VII.1 [LA-UR-11-11271]

Note: If the suite of benchmark cases changes, the correlation data (see Section 5 below) may need to be updated.

4.1 Output Data

This process determines the k_{eff} sensitivity coefficients for the benchmark models [LA-UR-14-23352; Sec. 3.1]. Sensitivity coefficients are calculated for the following reactions or parameters: elastic scattering, inelastic scattering, fission, capture [(n,2n), (n, γ), (n,p), (n,d), (n,t), (n, ^3He), (n, α)], fission total v, and fission χ [LA-UR-14-23352; Sec. 3.1] [LA-UR-14-26436; Sec. 3.4]. All other reactions are going to be minor to criticality safety and are ignored [LA-UR-14-26436; Sec. 3.4].

4.2 Input Data

The benchmark data is from criticality experiments that have been performed. These experiments determine the k_{eff} value (and associated uncertainty) for the fissile material configurations. Detailed information on each experiment configuration is required to develop the corresponding MCNP6 model. In some cases, a MCNP input file has already been developed for the experiment, e.g., ICSBEP has input files for many of their benchmarks.

4.3 Algorithm Description

The algorithm for the benchmarks is:

1. Determine the sensitivity coefficients for the benchmark models. (Corresponds to the first step of Section 3.3 above.)
2. Evaluate an application model to have Whisper calculate estimates of the uncertainty for the benchmark cases that have an unknown uncertainty (i.e., the variance, the square of the uncertainty, is less than 10^{-10}). A specific application model is not required for this step because only the Whisper-calculated benchmark uncertainties will be used.
3. Archive the benchmark library (TOC) file. (In the Whisper distribution, file `BenchmarkTOC.dat` was copied to `BenchmarkTOCNative.dat`.)
4. Manually edit the benchmark library (e.g., file `BenchmarkTOC.dat`) to replace the unknown uncertainties with the Whisper results.

For Whisper V1.0.0, the benchmark cases with an unknown uncertainty are:

- heu-met-fast-004-001, and
- ieu-met-fast-001-001, -002, -003, and -004.

4.4 Process Description

Like the application models, MCNP6 calculates the sensitivity values for the benchmark models. The Whisper program suite includes script files further simplify the process, but the process is complicated by the number of benchmarks (> 1000) to be evaluated. The execution and data flow for this process is shown in Figure 4-1⁵. At this time, Option 2 is appropriate for benchmark case LEU-COMP-THERM-60; the other benchmark cases can be evaluated by either option.

4.4.1 MCNP6 Input Files

In order to calculate the k_{eff} benchmark sensitivity data, the user must prepare MCNP6 input files for the benchmark models. The benchmark models must have the reference k_{eff} and uncertainty values, which are placed in a comment at the bottom of the MCNP6 input file:

```
c k(bmk) = [keff] +- [unc]
```

where `[keff]` and `[unc]` get replaced with the experimental values of k_{eff} and the uncertainty [LA-UR-14-26436; Sec. 3.1]. The manual edit step in Figure 4-1 replaces any nominally zero uncertainty values in the benchmarks with the uncertainty estimates calculated by Whisper. (The Whisper Fortran program calculates the benchmark experimental uncertainty when the variance (the square of the uncertainty) is less than 10^{-10} .)

The benchmark models must also have sensitivity parameters. There are two methods for including the sensitivity parameters in the MCNP6 input files.

4.4.1.1 Option 1

When using the script file RunMCNPInputs.csh (as shown in Figure 4-1), the MCNP6 input files must follow the following rules [LA-UR-14-26436; Sec. 2.3]:

1. The input file must contain the `kcode` card.
2. The input file may not contain `prdmp`, `kopts`, or `ksen` cards.

⁵ Figure 4-1 omits the energy grid data file (see Figure 3-1) for space reasons.

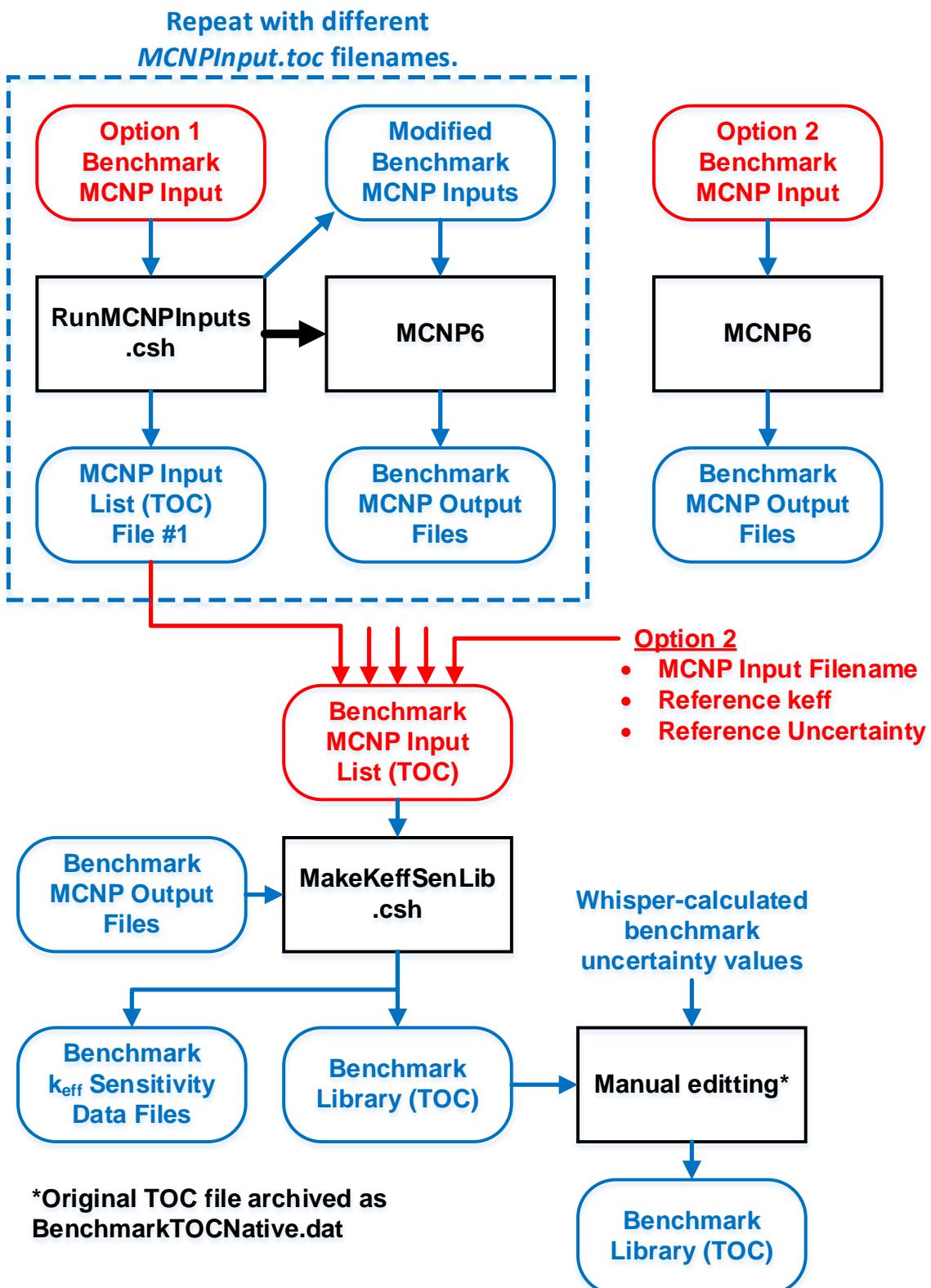


Figure 4-1
Benchmark Evaluation Flowchart

4.4.1.2 Option 2

If the script file RunMCNPInputs.csh is not used (as shown in Figure 4-1), the MCNP6 input files must have the following lines (except as noted below):

```
kcode 100000 1.0 100 600
kopts blocksize = 5
ksenl xs
rxn = +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
erg = 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
      4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
      2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
      4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
      6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
      3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
      1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
      6.4340e+00 8.1873e+00 2.0000e+01
prdmp j 9999999
```

For benchmark case LEU-COMP-THERM-60, the total number of cycles should be reduced to 300 because the geometric detail in the MCNP6 model results in very long run times [LA-UR-14-23352; Sec. 3.1]. Because the standard inputs are not used for LEU-COMP-THERM-60, LEU-COMP-THERM-60 must be evaluated with Option 2.

4.4.2 Command Lines

To evaluate the benchmark models, the user needs to execute the RunMCNPInputs.csh script file (Option 1) or MCNP6 (Option 2).

For Option 1, the user executes the RunMCNPInputs.csh script file in the directory where the benchmark model input files are located. The command syntax is:

```
> RunMCNPInputs.csh [walltime hh:mm:ss] MCNPInput.toc inp1
[inp2] ...
```

Each time the RunMCNPInputs.csh script file is executed, the filename for the MCNPInput.toc parameter must be different. See Section 3.5.2.1 above for additional information on the parameters.

For Option 2, the MCNP6 input files must be in the ‘Calcs’ subdirectory of the benchmark directory. The user then manually executes MCNP6.

For each benchmark case, verify the source has converged [LA-UR-14-23352; Sec. 3.1].

After all of the benchmark cases have been evaluated by MCNP6, the user must create the benchmark MCNP input list (table of contents) from the script file RunMCNPInputs.csh output files and the information for the Option 2 cases. The record format of the MCNP input list (table of contents) is:

1. MCNP6 input filename (without the directory path)
2. Benchmark reference k_{eff}
3. Benchmark reference uncertainty

The MakeKeffSenLib.csh script file is executed to create the benchmark library and the k_{eff} sensitivity data files. The command syntax is:

```
> MakeKeffSenLib.csh MCNPInput.toc KeffLib.toc
```

where

- | | |
|----------------------|--|
| <i>MCNPInput.toc</i> | = input file listing the MCNP6 input files and any benchmark k_{eff} values and uncertainties that are provided in the MCNP6 input files (required). |
| <i>KeffLib.toc</i> | = name of the sensitivity library that will be used by Whisper. |

4.5 Computer Programs

4.5.1 Script File RunMCNPIinputs.csh

The script file RunMCNPIinputs.csh, including the verification and validation, is described in Section 3.5.2 above.

4.5.2 Script File MakeKeffSenLib.csh

The script file MakeKeffSenLib.csh is described in Section 3.5.4 above. In this process, script file MakeKeffSenLib.csh was used to create the benchmark library file and the benchmark sensitivity data files. The benchmark library file distributed with the Whisper program suite is Whisper/Benchmarks/TOC/BenchmarkTOC.dat. The benchmark sensitivity data files distributed with the Whisper program suite are in directory Whisper/Benchmarks/Sensitivities. The only significant difference from Section 3.5.4 above is the contents of the benchmark library file, which contains:

1. MCNP6 input filename (without the directory path)
2. Benchmark reference k_{eff} (from the MCNP Input List file)
3. Benchmark reference uncertainty (from the MCNP Input List file)
4. Benchmark model calculated k_{eff} (from the MCNP6 output file; on the line with the test string “final estimated”)
5. Benchmark model calculated uncertainty (from the MCNP6 output file; on the line with the test string “final estimated”)

The verification and validation of script file MakeKeffSenLib.csh is described in Section 3.5.4.

5. Benchmark Experimental Correlation Data

5.1 Description

The Whisper program is capable of using the experimental correlation data for the benchmarks. The correlation values distributed with Whisper V1.0.0 were taken from the ICSBEP⁶ Handbook (via the Database for ICSBEP, DICE⁷, which is distributed with the Handbook) [LA-UR-14-26558; Sec. IV.B] and manually entered into a data file (Benchmark/Correlations/BenchCorrel.dat). In cases where two one-sided (i.e., asymmetric) benchmark uncertainties are given, the larger of the two is assumed for conservatism [LA-UR-14-26558; Sec. IV.B]. The file lists one correlation per line and each line has the names of two benchmark input files followed by a correlation coefficient [LA-UR-14-26436; Sec. 4.1].

The data file only lists the correlations for the benchmark cases incorporated into Whisper. If additional ICSBEP cases are added to the Whisper benchmark cases, the correlation data may need to be updated.

5.2 V&V Activities

Verify contents of data file Benchmark/Correlations/BenchCorrel.dat match the ICSBEP Handbook. The contents of data file Benchmark/Correlations/BenchCorrel.dat are listed in Appendix E.

LA-UR-14-26558 Ref. 24 states DICE (<https://www.oecd-nea.org/science/wpnics/icsbep/dice.html>) was accessed on Apr. 18, 2014. From this date, it was determined that the September 2013 Edition of DICE⁸ was used as input to Whisper. For this report, the September 2013 Edition of DICE was downloaded from <http://ncsp.llnl.gov/ICSBEP/> on December 22, 2014. The DICE correlation matrix is displayed in Appendix F.

5.3 Comparison

On December 22, 2014, the following differences between the data file Benchmark/Correlations/BenchCorrel.dat and the correlation matrix in the September 2013 Edition of DICE were identified:

1. Line 2:

heu-met-fast-020-002.i	heu-met-fast-031-001.i	0 .4600
------------------------	------------------------	---------

The correlation matrix does not include heu-met-fast-020-002 (HMF020-002). Instead, the matrix has HMF020-001, which is not a case in the Whisper benchmarks.

⁶ International Criticality Safety Benchmark Evaluation Project (ICSBEP)

⁷ Database for the International Handbook of Evaluated Criticality Safety Benchmark Experiments

⁸ Revision 5 of the DICE User's Manual (document NEA/NSC/DOC(95)03/II) was issued on September 30, 2013. Revision 6 was issued on September 30, 2014.

2. Line 99:

heu-sol-therm-013-001.i	heu-sol-therm-043-001.i	0.3500
-------------------------	-------------------------	--------

In the matrix, the correlation value for this pair is zero (blank entry). This value is instead for column header HST042-008, which would make the second case in the line above heu-sol-therm-042-008.

3. Line 100:

heu-sol-therm-013-001.i	heu-sol-therm-043-002.i	0.1100
-------------------------	-------------------------	--------

In the matrix, the correlation value for this pair is zero (blank entry). This value is instead for column header HST043-003, which would make the second case in the line above heu-sol-therm-043-003.

XCP-3 (private communication, Forrest Brown, 1/16/15) evaluated these differences.

1. In the 2013 ICSBEP Handbook, there are 2 models described in detail for heu-met-fast-020. They are not numbered as “case 001” and “case 002”, but rather as “detailed” and “simplified”. Both models have assumptions and uncertainties, but these are discussed and are small compared to the experiment uncertainty.

The input file for heu-met-fast-020-002.i is the simplified model from the ICSBEP Handbook. Presumably, the detailed model is the 001 case, which we do not have or use. It is perfectly reasonable to assume that the correlation data for the simple and detailed models is the same, or at least close enough that any impact on the Whisper results is negligible. The simple & detailed models have the same basic geometries and materials. This item is not a concern or issue.

2. Yes, this is a discrepancy that should be corrected as suggested.
3. Yes, this is a discrepancy that should be corrected as suggested.

Issues 2 and 3 above have the potential for influencing previously calculated results (e.g., the USLs in LA-UR-14-23352, NCS-TECH-14-019, and NCS-TECH-14-031). XCP-3 reported that the significance and impact of these 2 errors should be negligible because the correlation data is used only in the rejection of benchmarks. Other than the rejection process to exclude benchmarks from further consideration, the correlation data is not used in calculating the calculational margin value. Expert judgment (by Kiedrowski and Brown) is that the Whisper results to date are reliable, that the errors described above should have little or no impact, and that there is no compelling need to rerun everything. Appendix A of LA-UR-14-23352 lists the Whisper benchmarks and identifies the rejected benchmarks (with red text). The four benchmarks:

- heu-sol-therm-042-008
- heu-sol-therm-043-001
- heu-sol-therm-043-002

- heu-sol-therm-043-003

are all listed and not rejected, therefore, the incorrect correlation data did not result in any erroneous benchmark rejections. This issue is identified in a problem report (NCS-SQM-WHISPER-PROBID01) in order to initiate corrective actions.

5.4 V&V Results

6. Reject Inconsistent Benchmark Cases

The fundamental premise of the Whisper program is that uncertainties in the nuclear data are the primary source of computational bias. In practice, this is not true for every benchmark case. This process determines for each benchmark cases whether the uncertainties in the nuclear data are the primary source of computational bias. If the computational bias cannot be reduced through a consistent adjustment of the nuclear data, the benchmark is placed on the list of rejected benchmarks. [LA-UR-14-23352; Sec. 3.1]

6.1 Output Data

In addition to the normal report, Whisper creates a data file listing the MCNP6 input filename for the rejected benchmark cases.

6.2 Input Data

For this process, the k_{eff} sensitivity data for the benchmark cases must be available. The benchmark sensitivity data distributed with the Whisper program can be used, or the user can create their own.

The benchmark correlation data is not required but is strongly recommended [LA-UR-14-26436; Sec. 4.2]. The $-k$ argument will cause Whisper to consider the experimental correlations during the GLLS nuclear data adjustment.

6.3 Algorithm Description

The generalized linear least squares (GLLS) method is used to adjust the nuclear data to minimize the chi-squared statistic (see LA-UR-14-23202, eq. 10). Benchmarks are iteratively rejected until the chi-squared value divided by the number of benchmarks is less than the maximum limit (default value is 1.2). [LA-UR-14-23352; Sec. 3.1]

6.4 Process Description

The Whisper program is used (with the $-r$ option and preferably the $-k$ option) to create the rejected benchmark data. The data flow for creating the list of rejected benchmarks is shown in Figure 6-1.

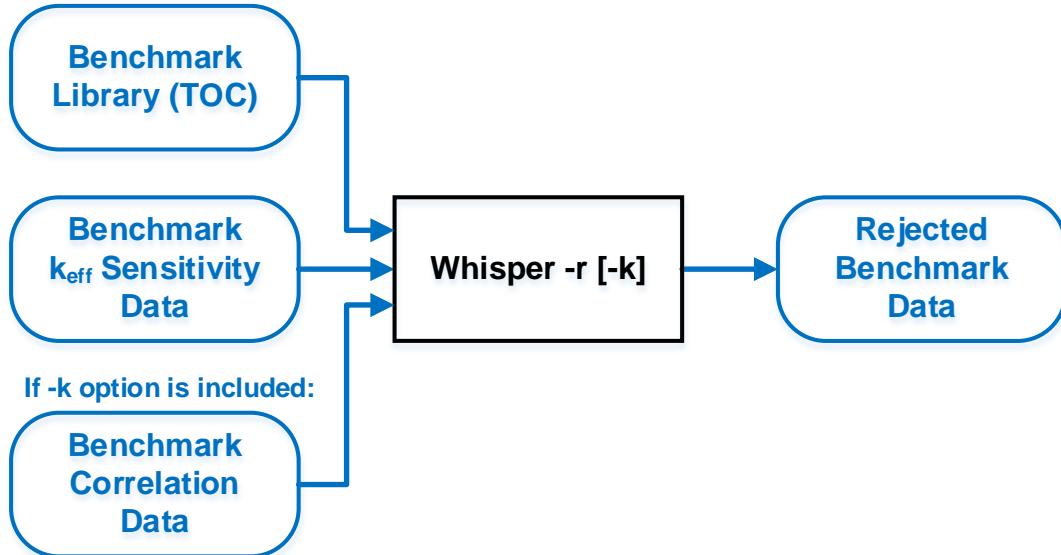


Figure 6-1
Benchmark Rejection Flowchart

6.5 Computer Programs

6.5.1 Whisper Program

6.5.1.1 Command Syntax

The Whisper code has several possible command line arguments; see Table I of LA-UR-14-26436 for the full list. The command to reject inconsistent benchmark cases has the format:

```
> whisper -r RejectedBenchmarks.dat [-k Correlations.dat]
```

where

RejectedBenchmarks.dat = output filename where the rejected benchmarks will be listed.

Correlations.dat = name of the input file for the correlation data.

The benchmark correlation data is not required but is strongly recommended [LA-UR-14-26436; Sec. 4.2].

6.5.1.2 V&V Activities

A thorough review of the Whisper source code was performed. The *Whisper Source Code Inspection Report* explains how and where the LA-UR-14-26558 equations and algorithms were implemented in the Whisper source code.

7. Covariance Data Processing

Whisper requires nuclear covariance data to compute the baseline USLs [LA-UR-14-26436; Sec. 3.5]. The Whisper program suite is distributed with base and adjusted covariance data. This section explains how this data was generated.

The base covariance data does not need to be regenerated unless new or alternative covariance data (in COVERX format), i.e., other than the SCALE6.1 data, is available and selected for use. The script file ProcessCovData.csh is provided so future covariance data releases in the COVERX format may be processed for Whisper.

The Fortran program Whisper V1.0.0 makes certain assumptions related to the covariance data (for the thermal scattering kernel $\{S(\alpha, \beta)\}$ cross sections) based on the currently available SCALE-6 covariance data. See the *Whisper Source Code Inspection Report* for details related to the sensitivity factors for the $S(\alpha, \beta)$ cross sections. Because of this assumption, Whisper V1.0.0 may not be compatible with all (future) covariance data.

The adjusted covariance data does not need to be regenerated unless the base covariance, benchmark sensitivity, or benchmark correlation data changes. Unless the base covariance data has been replaced, it is not expected that a user will create the adjusted covariance data as given in this section. Instead, it is expected that users will use the process to calculate new covariance data (see Section 9 below). However, the two processes are similar in that they use the Whisper program to calculate the adjusted covariance data. Then, if an institution wishes to permanently use the new adjusted covariance data, it can be placed in the default directory (see Section 10).

7.1 Output Data

The covariance data is located in directory Whisper/CovarianceData.

7.1.1 Base Covariance Data

The base covariance data files have the same information as the native covariance data file (see Section 7.2 below) but the data has been parsed into separate files and reformatted.

The ‘Data’ subdirectory contains the base covariance data. The base covariance files have the name cov.ZA.dat where ZA is replaced by the appropriate ZA of the isotope, e.g., hydrogen is 1001. Thermal scattering laws have the ZA represented by the string used by MCNP, e.g., ‘lwtr’ for hydrogen bonded in water. [LA-UR-14-26436; Sec. 5.2]

7.1.2 Adjusted Covariance Data

The adjusted covariance data is calculated by Whisper from the base covariance data, the benchmark sensitivity data, and, preferably, the benchmark correlation data. The ‘Adjusted’ subdirectory contains the adjusted data files. The filenames have the same format as the base covariance files.

7.2 Input Data

The input data to this process is the 44-group covariance data from the SCALE6.1 code distribution, which was the most comprehensively available processed set available at the time. The ‘Native’ subdirectory contains the original, unprocessed file distributed with SCALE6.1. [LA-UR-14-26436; Sec. 3.5]

7.3 Algorithm Description

For the base covariance data, there is not an algorithm. There is only a process for removing information and headings irrelevant to Whisper [LA-UR-14-26436; Sec. 5.2] and parsing the native covariance data into separate isotope files.

For the adjusted covariance data, the algorithm is to calculate the adjusted or residual covariance matrix according to LA-UR-14-26558, eq. 41.

7.4 Process Description

The process for creating the base and adjusted covariance data is shown in Figure 7-1. The base and adjusted covariance data was calculated and included in the Whisper program suite. However, the ProcessCovData.csh script file is provided in the Whisper program suite so future covariance data releases in the COVERX format may be processed for Whisper [LA-UR-14-26436; Sec. 5.2].

After using Whisper to calculate new adjusted covariance data files, the new adjusted covariance directory may be incomplete because Whisper only prints out the covariance data files that were used in the benchmark suite for the nuclear covariance data adjustment. Script file CopyUnadjustedData.csh is used to complete the new adjusted covariance directory. For the isotopes missing in the adjusted covariance data directory, CopyUnadjustedData.csh copies the data file from the base covariance data directory.

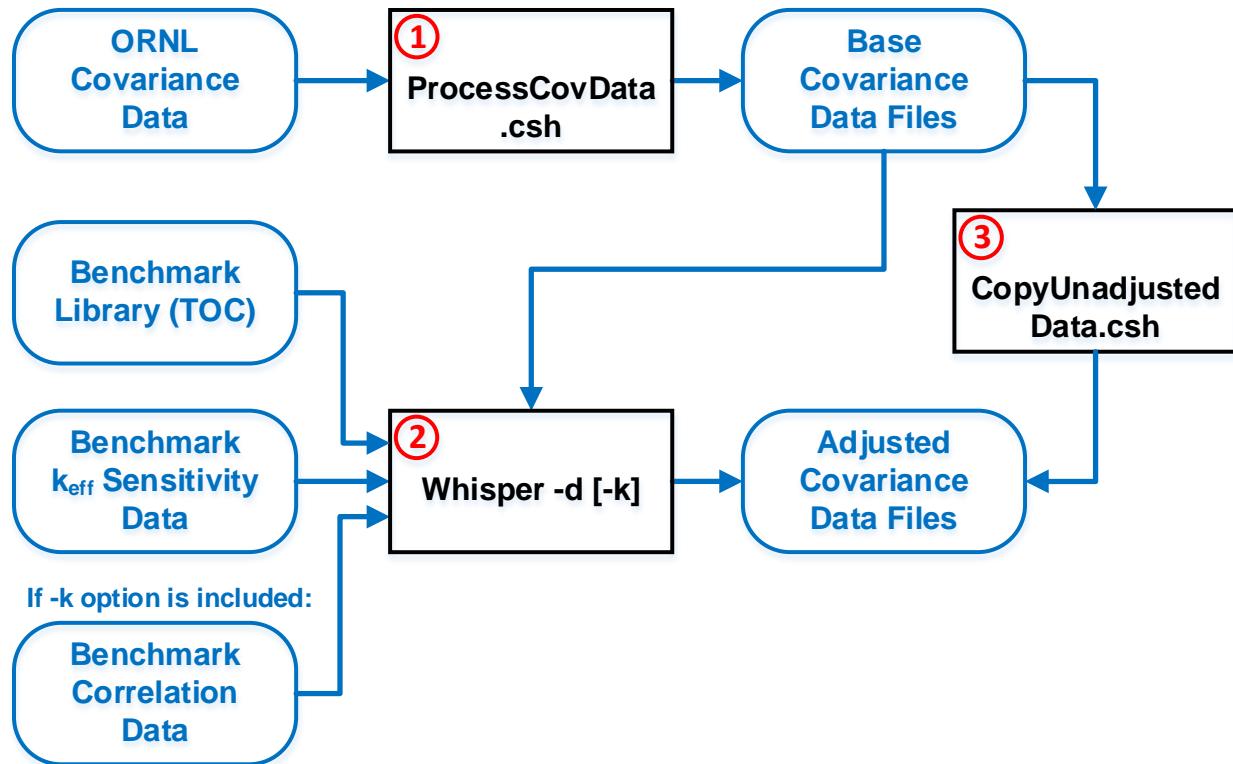


Figure 7-1
Covariance Data Processing Flowchart

7.4.1 Command Lines

The base covariance data files distributed in directory Whisper/CovarianceData/Scale6.1/Data were created by going to directory Whisper/CovarianceData/Scale6.1/Data and executing the command:

```
> ProcessCovData.csh Native/ORNL_SCALE6.1.cov
```

The adjusted covariance data files distributed in directory Whisper/CovarianceData/Scale6.1/Adjusted were created by going to directory Whisper/CovarianceData/Scale6.1/Adjusted and executing the command:

```
> whisper -d AdjCovDir -k Correlations.dat
```

To complete the adjusted covariance data, the CopyUnadjustedData.csh script file was executed from the Whisper/CovarianceData/Scale6.1 directory:

```
> CopyUnadjustedData.csh Base Adjusted
```

7.5 Computer Programs

7.5.1 Script File ProcessCovData.csh

7.5.1.1 Command Syntax

The syntax for script file ProcessCovData.csh is:

```
> ProcessCovData.csh coverx
```

where

coverx = covariance data file in COVERX format (required).

7.5.1.2 Operations

Script file ProcessCovData.csh performs the following:

1. Set variable NErg to the number of energy groups in the covariance data, i.e., from the line beginning with COVERX identifier “1d”, get the third value.

The format of a COVERX file is documented in Table M18.A.8 of ORNL/TM-2005/39.

2. Copy the covariance data energy grid to file EnergyGrid.dat. In the covariance data file, the energy grid is the block beginning with “3d”; the next block begins with “5d”. Do not include the COVERX identifier “3d”, i.e., replace “3d” with a blank string.
3. Parse the covariance data into individual files named with the SCALE ZAID.
 - a. Copy each block of covariance data to a separate output file, i.e., the first block beginning with COVERX identifier “7d” is written to file “out1”, the second to “out2”, etc.
 - b. Delete file “out” which is the text preceding the first “7d”.
 - c. Rename each output file to the format “tmp.ZA1.MT1.ZA2.MT2” where *ZA1* is the 6-digit numerical ZA identifier for the first isotope, *MT2* is the four-digit reaction identifier for the first isotope, etc.
 - d. For each *ZA1* value, create a covariance file named “cov.ZA1.dat”.
 - 1) Write *ZA1*, number of energy groups (NErg), and number of blocks of covariance data (i.e., number of filenames beginning with “tmp.ZA1”) on the first line.
 - 2) Write the energy grid by copying file EnergyGrid.dat to the covariance data file.
 - 3) Write a table listing *ZA1*, *MT1*, *ZA2*, and *MT2* (from each filename beginning with “tmp.ZA1”).

- 4) Copy each filename beginning with “tmp.ZA1” to the “cov.ZA1.dat” file.
 - 5) Delete the copied “tmp.ZA1” files.
4. Change the filenames with the following ZA identifiers to the MCNP6 S(α, β) identifiers to create covariance data for the MCNP6 S(α, β) models. Also change the ZA1 values in the files. These modifications are appropriate to use the ORNL covariance data with MCNP6; see Appendix G for the supporting documentation.

SCALE ZA Identifier	MCNP6 S(α, β) Identifier
1001	lwtr
1701	h-zr
1801	1001
1901	poly
1002	hwtr
1802	1002
4309	be
6312	grph

However, Whisper V1.0.0 is not using the correct covariance data for the meta-stable isotopes. The ORNL covariance data and MCNP6 cross section library use different identifiers for meta-stable isotopes. Script file ProcessCovData.csh does not modify the covariance data files for the meta-stable isotopes. Consequently, Whisper does not use the correct covariance data when evaluating a meta-stable isotope in an MCNP6 input file. Except for Am-242m, Whisper V1.0.0 does not use any covariance data with the meta-stable isotopes. For Am-242m ($t_{1/2} = 141$ y), which has the ZA identifier 95242 in MCNP6 for historical reasons, Whisper V1.0.0 uses the covariance data for Am-242 ($t_{1/2} = 16.02$ h). See Appendix G for additional information.

5. Remove the COVERX identifiers, i.e., replace “7d”, “8d”, and “9d” with blank strings.

7.5.1.3 V&V Activities

Script file ProcessCovData.csh can be verified and validated by:

1. a review of the script file, and
2. comparing the base covariance data file to the native covariance data file.

7.5.1.3.1 Script File Review

The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	7
2.	9 – 22
3.	24 – 71
3.a	24 – 25
3.b	26
3.c	28 – 42
3.d	44 – 71
3.d.1	60
3.d.2	61
3.d.3	62 – 68
3.d.4	69
3.d.5	70
4.	73 – 81
5.	94 – 100

7.5.1.3.2 Covariance Data Files Comparison

Excerpts of the base covariance data file ‘cov.lwtr.dat’ are listed in Appendix H. Excerpts of the native covariance data file ‘ORNL_SCALE6.1.cov.’ are listed in Appendix I. The two files (Appendices H and I) were compared in Appendix J. Remember script file ProcessCovData.csh renames the file originally created as ‘cov.1001.dat’ to ‘cov.lwtr.dat’. Script file ProcessCovData.csh also changes the material identification from “1001” to “lwtr”. Other than the intentional change in material identification, no discrepancies between the two files were identified.

7.5.1.3.3 Reaction Number Cross Reference

Script File ProcessCovData.csh removes information and headings irrelevant to Whisper and parses the native covariance data into separate isotope files. The native covariance data contains reaction (MT) numbers used by SCALE6.1. The covariance data files used by Whisper contain the same reaction numbers. Because SCALE6.1 and MCNP6 sometimes use different identifiers for isotopes, it is prudent to ask if SCALE6.1 and MCNP6 have any differences in the reaction numbering schemes.

The following table lists the relevant reaction (MT) numbers (i.e., used by Whisper) and the definitions in SCALE6.1 and MCNP6. The SCALE6.1 covariance data contains many other reactions, but the data for the reaction numbers not listed is ignored by Whisper. For each reaction number, the SCALE6.1 and MCNP6 reactions are identical.

Relevant Reaction (MT) Number	SCALE6.1 Definition [ORNL/TM-2005/39; Table M18.1.4]	MCNP6 Definition [LA-CP-13-00634; Table 3-104]
2	Elastic scattering	Elastic
4	Inelastic scattering	Total Inelastic
16	n,2n	(n,2n)
18	Fission	Total Fission
102	n, γ	(n, γ)
103	n,p	(n,p)
104	n,d	(n,d)
105	n,t	(n,t)
106	n, ${}^3\text{He}$	(n, ${}^3\text{He}$)
107	n, α	(n, α)
452	$\bar{\nu}$	Total Fission ν
1018	χ	Total Fission Chi

7.5.1.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

However, script file ProcessCovData.csh (Whisper V1.0.0) has an omission; it fails to adjust the correct covariance data for the meta-stable isotopes. See Section 7.5.1.2 above and Appendix G for additional information.

No unintentional discrepancies between the base covariance data file ‘cov.lwtr.dat’ (Appendix H) and the native covariance data file ‘ORNL_SCALE6.1.cov’ (Appendix I) were identified in Appendix J.

The definition of the reaction (MT) numbers used by Whisper is consistent between SCALE and MCNP6.

7.5.2 Whisper Program

7.5.2.1 Command Syntax

The Whisper code has several possible command line arguments; see Table I of LA-UR-14-26436 for the full list. The command line for creating the adjusted covariance data is:

```
> whisper -d AdjCovDir [-k Correlations.dat]
```

where

- AdjCovDir* = previously created directory where the adjusted covariance data files will be placed (required).
- Correlations.dat* = name of the input file for the correlation data (optional).

The benchmark correlation data is not required but is strongly recommended [LA-UR-14-26436; Sec. 4.2].

7.5.2.2 Operations

For covariance data processing, Whisper performs the following operations:

1. Calculate the covariance matrix of the relative difference vector according to LA-UR-14-26558, eq. 40.
2. Calculate the adjusted or residual covariance matrix according to LA-UR-14-26558, eq. 41.
3. Write the adjusted covariance data (for use in subsequent runs of Whisper).

For the adjusted covariance data, the algorithm is to calculate the adjusted or residual covariance matrix according to LA-UR-14-26558, eq. 41.

7.5.2.3 V&V Activities

A thorough review of the Whisper source code was performed. The *Whisper Source Code Inspection Report* explains how and where the LA-UR-14-26558 equations and algorithms were implemented in the Whisper source code.

7.5.3 Script File CopyUnadjustedData.csh

7.5.3.1 Command Syntax

The syntax to execute CopyUnadjustedData.csh is [LA-UR-14-23352; Sec. 5.1]:

```
> CopyUnadjustedData.csh BaseDir NewAdjustedDir
```

where

- BaseDir* = the directory containing the base nuclear covariance data (required).
- NewAdjustedDir* = the directory containing the new adjusted covariance data (required).

7.5.3.2 Operations

Script file CopyUnadjustedData.csh (in directory Whisper/Utilities/CovarianceData) performs the following:

1. Verifies that two (and only two) arguments are on the command line.
2. Verifies the directory for the base covariance data exists.
3. Verifies the directory for the new adjusted covariance data exists.
4. For each file in the base covariance data directory:
 - a. If the adjusted covariance data directory does not have a file with the same name, copy the base covariance data file to the adjusted covariance data directory.

7.5.3.3 V&V Activities

Script file CopyUnadjustedData.csh can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	3 – 7
2.	12 – 15
3.	16 – 19
4.	21 – 27

7.5.3.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

8. Append New Benchmark Cases

If new experimental benchmark data becomes available, this process can add the new k_{eff} sensitivity data file to the existing data file (without re-evaluating the prior cases). The script file created for this process automatically replaces the current benchmark library file with the updated library file.

If the new benchmark k_{eff} sensitivity data file has replaced the current sensitivity data for evaluations, i.e., is the data file selected by the WHISPER_BENCHMARK_TOC environment variable, the installation tests should now be rerun (see Section 12 below) as it may change reference solutions. If it does, the user should verify this change is desired and update the installation test reference solutions (see Section 11 below). [LA-UR-14-23352; Sec. 6.2]

Note: If the suite of benchmark cases changes, the correlation data (see Section 5 above) may need to be updated.

8.1 Output Data

This process determines the k_{eff} sensitivity coefficients for new benchmark models and adds them to the existing benchmark cases.

8.2 Input Data

The benchmark data is from criticality experiments that have been performed. These experiments determine the k_{eff} value (and associated uncertainty) for the fissile material configurations. Detailed information on each experiment configuration is required to develop the corresponding MCNP6 model.

8.3 Algorithm Description

New benchmark k_{eff} sensitivity data is appended to the current data by the following steps:

1. Determine the sensitivity coefficients for the benchmark models [LA-UR-14-23352; Sec. 6.2].
2. Append the new sensitivity coefficients to the current benchmark sensitivity data [LA-UR-14-23352; Sec. 6.2].

8.4 Process Description

The sensitivity coefficients for the benchmark models are calculated by MCNP6. Figure 8-1 shows how the script files can be used to create the data files appropriate for Whisper. This part of the process is similar to the application and benchmark models evaluations (Section 3.4 and 4.4).

The script file AppendBenchmarks.csh (in directory Whisper/Utilities/Benchmarks) will append the new sensitivity coefficients to the current sensitivity coefficients. Figure 8-2 illustrates this step.

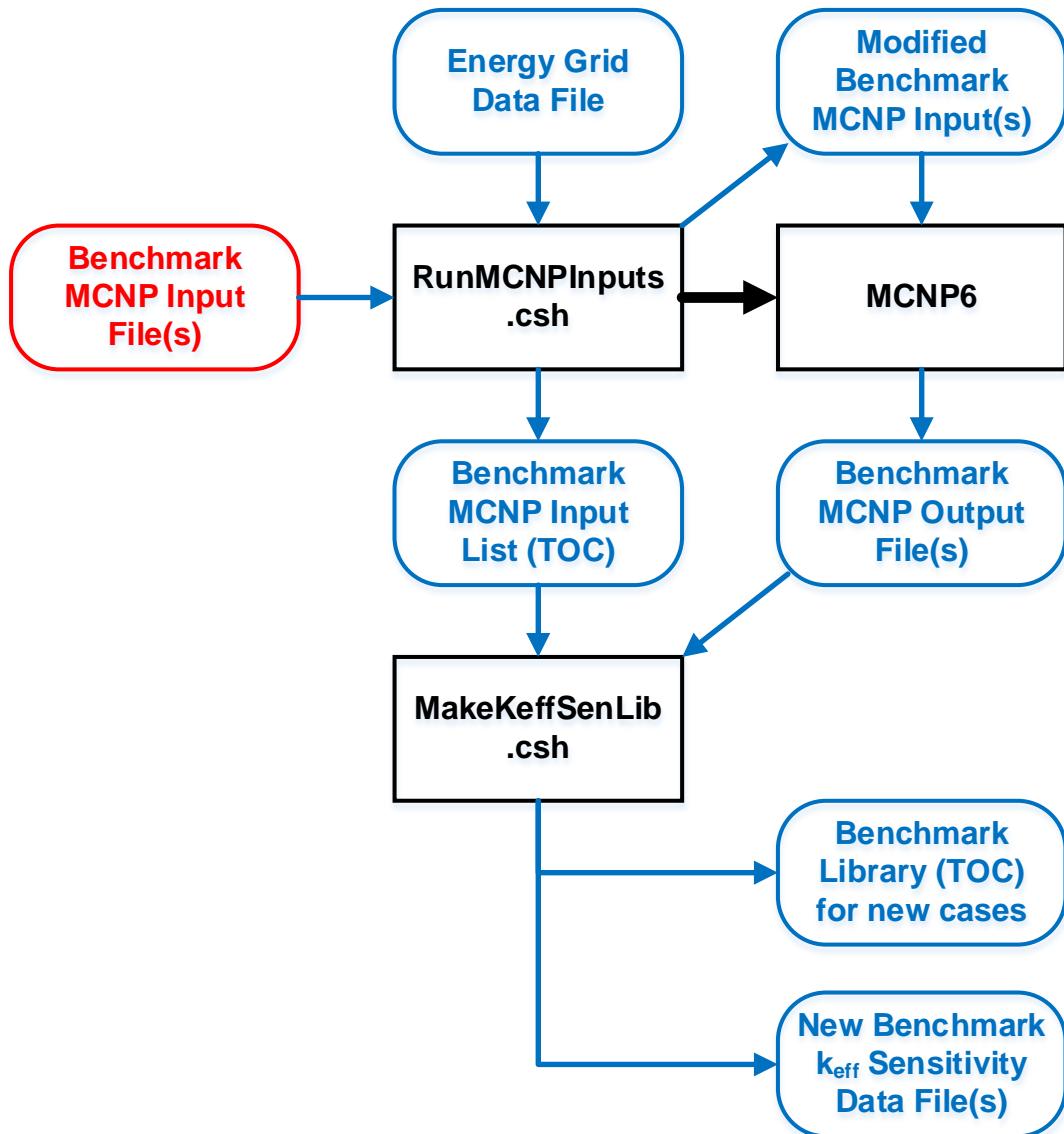


Figure 8-1
Append New Benchmark Flowchart

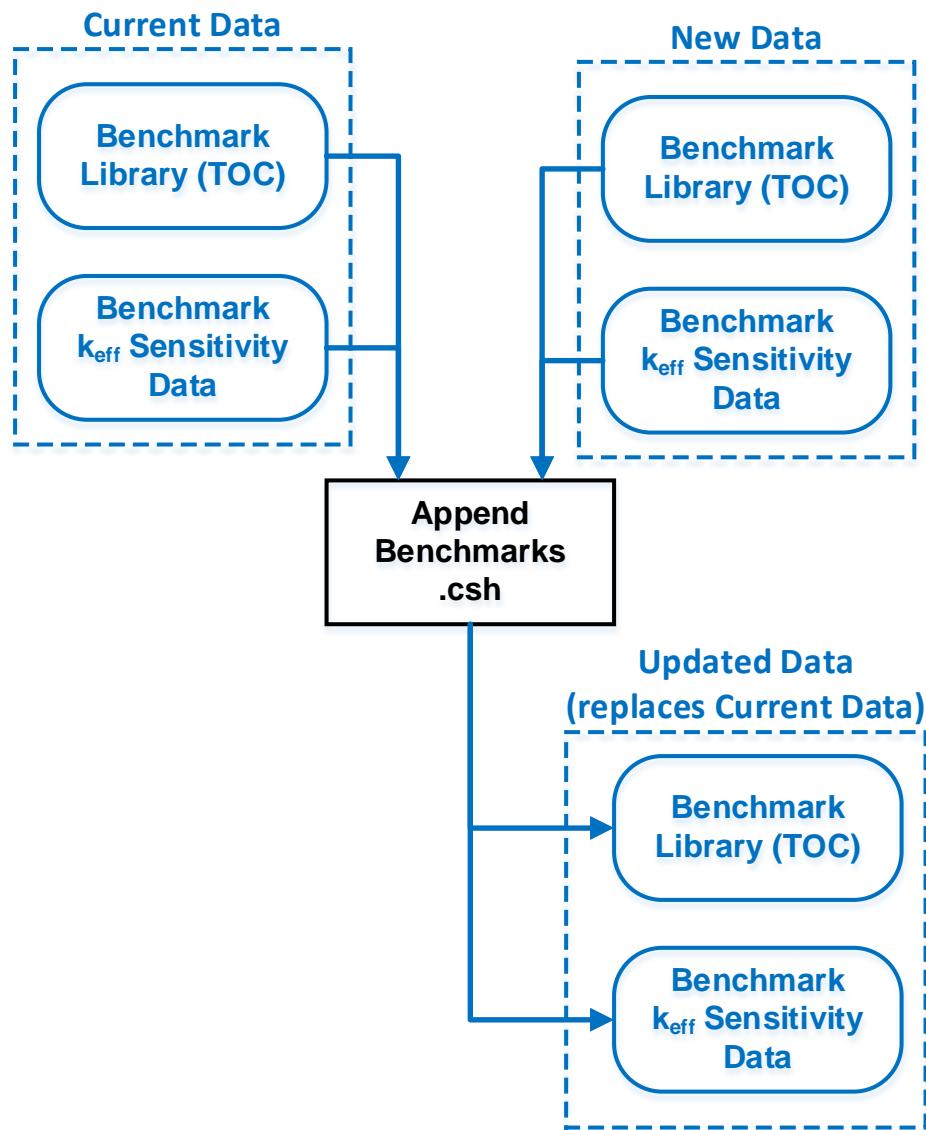


Figure 8-2
Append New Benchmark Flowchart

8.4.1 MCNP6 Input Files

In order to append new benchmark cases to the current benchmark k_{eff} sensitivity data, an MCNP6 model must be developed from the new experimental data. In addition, the new benchmark cases must be developed in a directory other than the current sensitivity data directory. The benchmark k_{eff} and uncertainty are placed in a comment at the bottom of the MCNP6 input file:

```
c k(bmk) = [keff] +- [unc]
```

where $[keff]$ and $[unc]$ get replaced with the experimental values of k_{eff} and the uncertainty [LA-UR-14-26436; Sec. 3.1].

Because this process uses script file RunMCNPInputs.csh, the MCNP6 input files must follow the following rules:

1. The input file must contain the kcode card.
2. The input file may not contain prdmp, kopts, or ksen cards.

The process can be performed without script file RunMCNPInputs.csh, but the user will have to perform the tasks that have been automated in the script file; see Option 2 in Section 4.4 above.

8.4.2 Command Lines

The command lines for this process are:

```
> RunMCNPInputs.csh [walltime hh:mm:ss] MCNPInput.toc inp1  
[inp2] ...  
  
> MakeKeffSenLib.csh MCNPInput.toc New.toc  
  
> AppendBenchmarks.csh Current.toc New.toc
```

where

- MCNPInput.toc* = input file listing the MCNP6 input files and any benchmark k_{eff} values and uncertainties that are provided in the MCNP6 input files (required).
- New.toc* = the name of the benchmark library for the new benchmark cases (required).
- Current.toc* = the name of the current benchmark library which is overwritten with the updated benchmark library (required).

8.5 Computer Programs

8.5.1 Script File RunMCNPIInputs.csh

The script file RunMCNPIInputs.csh, including the verification and validation, is described in Section 3.5.2 above.

8.5.2 Script File MakeKeffSenLib.csh

The use of script file MakeKeffSenLib.csh with benchmark cases is described in Section 4.5.2 above.

8.5.3 Script File AppendBenchmarks.csh

8.5.3.1 Command Syntax

The syntax to execute AppendBenchmarks.csh is [LA-UR-14-23352; Sec. 6.2]:

```
> AppendBenchmarks.csh Current.toc New.toc
```

where

Current.toc = the name of the current benchmark library which is overwritten with the updated benchmark library (required).

New.toc = the name of the benchmark library for the new benchmark cases (required).

8.5.3.2 Operations

Script file AppendBenchmarks.csh performs the following:

1. Check whether two arguments (current and new benchmark library filenames) were provided.
2. Verify that the current and new benchmark library files exist.
3. Because this is a permanent change that can only be undone by a reinstall of Whisper, the user is requested to type confirm [LA-UR-14-23352; Sec. 6.2].
4. If the user enters “confirm”
 - a. Get the directory for the current benchmark data files from the first line of the current benchmark library file.
 - b. Get the directory for the new benchmark data files from the first line of the new benchmark library file.
 - c. Verify that the directories for the current and new benchmark data files exist.

- d. For each benchmark in the new library file (i.e., for the second and subsequent lines):
 - 1) Get the benchmark name.
 - 2) Append ‘k’ to the benchmark name to have the filename of the new benchmark data.
 - 3) Verify the new benchmark data file exists in the directory for the new benchmarks.
 - 4) Verify the new benchmark data file does not exists in the directory for the current benchmarks.
- e. Verify the file ‘TempTOCFile.tmp’ does not exist.
- f. Copy the new benchmark names (the second and subsequent lines of the new library file) to the file ‘TempTOCFile.tmp’.
- g. Verify the file ‘NewTOCFile.tmp’ does not exist.
- h. Create the updated library information by copying the current benchmark library and the new benchmark names (file ‘TempTOCFile.tmp’) to the file ‘NewTOCFile.tmp’.
- i. Change the file system authorities to allow the script to write to the current benchmark data directory and the library file.
- j. For each benchmark in the new library file (i.e., for the second and subsequent lines):
 - 1) Get the benchmark name.
 - 2) Append ‘k’ to the benchmark name to have the filename of the new benchmark data.
 - 3) Copy the new benchmark sensitivity data file to the current benchmark data directory.
 - 4) Change the file system authority to protect the copied file from user changes.
- k. Rename file ‘NewTOCFile.tmp’ to the current benchmark library filename.
- l. Change the file system authority to protect the current benchmark library file from user changes.

8.5.3.3 V&V Activities

Script file AppendBenchmarks.csh can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	5 – 11
2.	16 – 23
3.	25 – 34
4.	36 – 111
4.a	38
4.b	39
4.c	40 – 47
4.d	49 – 65
4.d.1	53
4.d.2	54
4.d.3	55 – 58
4.d.4	59 – 63
4.e	69 – 72
4.f	73 – 74
4.g	78 – 81
4.h	82
4.i	86 – 87
4.j	88 – 96
4.j.1	90
4.j.2	91
4.j.3	92
4.j.4	94
4.k	99
4.l	100

8.5.3.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

9. Create New Covariance Directory and Data

This section explains how to create a new directory of covariance data. This process can incorporate new benchmark sensitivity or benchmark correlation data into the (adjusted) covariance data. The user can then use the new covariance data by either using the -c argument on the Whisper command line or setting the environment variable

WHISPER_COVDATA_PATH to the new covariance data directory [LA-UR-14-23352;

Sec. 5.1]. Alternatively, the new covariance data can be placed in the default directory (see Section 10 below).

9.1 Output Data

This process creates a new directory containing a copy of the base covariance data and new adjusted covariance data. Any changes to the adjusted covariance data depend on the changes made to the benchmark k_{eff} sensitivity data and/or the benchmark correlation data.

9.2 Input Data

The input for this process, creating a new covariance directory and data, is new benchmark k_{eff} sensitivity data and/or new benchmark correlation data. (This process is only necessary if new benchmark sensitivity or benchmark correlation data is available.)

9.3 Algorithm Description

To create new covariance data, e.g., user covariance data:

1. Create a directory for the new covariance data. Subdirectories ‘Data’ and ‘Adjusted’ are required for the base and adjusted covariance data.
2. Copy the base covariance data files to the new base covariance data directory.
3. Use Whisper to calculate the new adjusted covariance data files.

Whisper only prints out the covariance data files that were used in the benchmark suite for the nuclear covariance data adjustment. Therefore, this step results in an incomplete adjusted covariance data.

4. For the isotopes that were not calculated, copy the covariance data files from the base directory to the adjusted directory.

9.4 Process Description

Figure 9-1 illustrates the process of creating a new covariance directory and data. The steps of creating the directories and copying the base covariance data, Steps 1 and 2 above, are performed manually. Step 3, calculating new adjusted covariance data, is performed with Whisper (with the `-d` option and preferably the `-k` option). Step 4 is performed with the script file `CopyUnadjustedData.csh`, which is described below. These programs are discussed in Section 7 above.

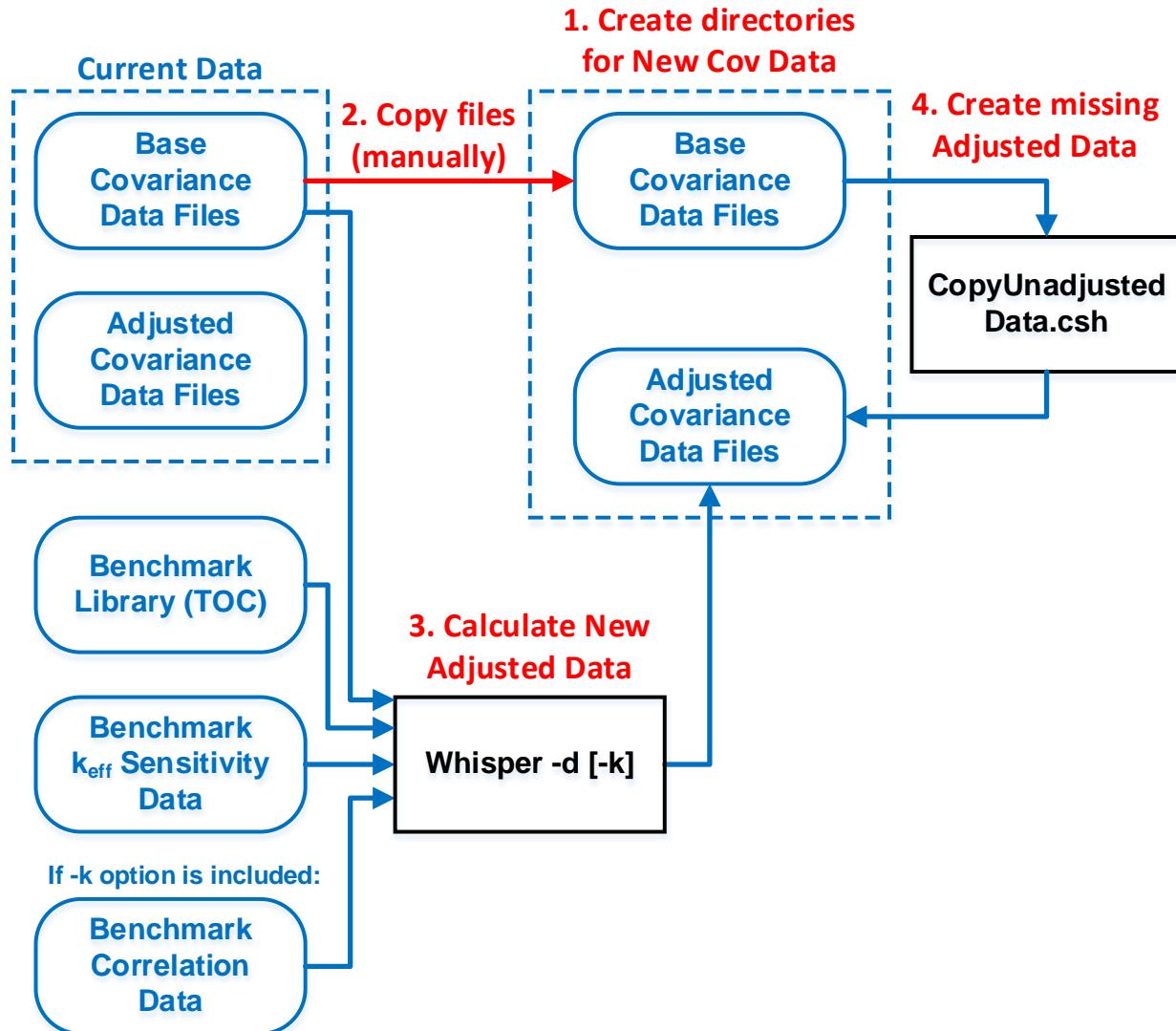


Figure 9-1
Create New Covariance Directory and Data Flowchart

9.5 Computer Programs

9.5.1 Whisper Program

The use of Whisper in calculating adjusted covariance data is discussed in Section 7.5.2 above.

9.5.2 Script File CopyUnadjustedData.csh

After using Whisper to calculate new adjusted covariance data files, the new adjusted covariance directory may be incomplete because Whisper only prints out the covariance data files that were used in the benchmark suite for the nuclear covariance data adjustment. Script file CopyUnadjustedData.csh is used to complete the new adjusted covariance directory. For the

isotopes missing in the adjusted covariance data directory, CopyUnadjustedData.csh copies the data file from the base covariance data directory.

The use of script file CopyUnadjustedData.csh in completing the adjusted covariance data directory is discussed in Section 7.5.3 above.

10. Replace Default Covariance Data

If an institution wishes to permanently use a new set of adjusted covariance data, use this process to copy the new adjusted covariance data to the default directory (Whisper/CovarianceData/SCALE6.1/Adjusted), thereby replacing the previous adjusted covariance data. [LA-UR-14-23352; Sec. 5.1]

Users should be aware that is a permanent change to the Whisper distribution users are strongly encouraged to make a backup of the Whisper/CovarianceData/SCALE6.1/Adjusted directory. Note that the installation tests will also no longer match the reference values if this is done, so the user should check and update those. The original adjusted covariance data can be restored by reinstalling Whisper, which may clear out other changes. [LA-UR-14-23352; Sec. 5.1]

10.1 Output Data

This process replaces the adjusted covariance data in the default directory Whisper/CovarianceData/SCALE6.1/Adjusted.

10.2 Input Data

This process requires new adjusted covariance data files. The new data files must be in a directory other than the default directory (Whisper/CovarianceData/SCALE6.1/Adjusted).

10.3 Algorithm Description

There is not an algorithm for replacing the default covariance data, only a process which is described below.

10.4 Process Description

The steps to replace the default covariance data are:

1. Copy the directory of new adjusted covariance data to the default directory (Whisper/CovarianceData/SCALE6.1/Adjusted).
 - a. This deletes all of the old adjusted covariance data.
2. If the adjusted covariance data does not exist for an isotope which has base covariance data, copy the base covariance data file to the adjusted covariance data directory.

10.5 Computer Programs

10.5.1 Script File UpdateCovariance.csh

10.5.1.1 Command Syntax

The syntax to execute UpdateCovariance.csh is [LA-UR-14-23352; Sec. 5.1]:

```
> UpdateCovarianceData.csh NewAdjustedData
```

where

NewAdjustedData = the directory name for the new adjusted covariance data (required).

10.5.1.2 Operations

Script file UpdateCovariance.csh (in directory Whisper/Utilities/CovarianceData) performs the following:

1. Verifies that one (and only one) argument is on the command line.
2. Verifies the directory for the new adjusted covariance data exists.
3. Because this is a permanent change that can only be undone by a reinstall of Whisper, the user is requested to type confirm [LA-UR-14-23352; Sec. 5.1].
4. If the user enters “confirm”:
 - a. Change the file system authorities to allow the script to overwrite the old adjusted covariance files.
 - b. Copy the directory of new adjusted covariance data to the default directory (Whisper/CovarianceData/SCALE6.1/Adjusted).
 - c. For each file in the base covariance data directory (Whisper/CovarianceData/SCALE6.1/Data):
 - 1) If the adjusted covariance data directory does not have a file with the same name, copy the base covariance data file to the adjusted covariance data directory.
 - d. Change the file system authorities to protect the adjusted covariance data from user changes.

10.5.1.3 V&V Activities

Script file UpdateCovariance.csh can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	3 – 6
2.	8 – 12
3.	14 – 21
4.	23 – 58
4.a	29 – 32
4.b	33
4.c	40 – 46
4.d	48 – 49

10.5.1.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

11. Updating Installation Test Reference Solutions

Upon changing the Whisper directory structure by adding benchmarks, changing covariance data, etc., the reference installation test solutions may change. These changes should intentional and should be judged by the user to be what they expect. If this is so, the reference files may be updated. Following the update, the installation tests allow users to verify that future changes do not have unintentional effects. [LA-UR-14-23352; Sec. 6.3]

11.1 Output Data

This process replaces the reference test solutions (output files) in directory Whisper/Testing/Installation.

11.2 Input Data

No special input is required to update the installation test reference solutions. Only the installation test input (see Section 12.2 below) is used.

11.3 Algorithm Description

There is not an algorithm for updating installation test reference solutions, only a process which is described below.

11.4 Process Description

The process for updating the test reference solutions is:

1. Run the installation tests.
2. Overwrites the reference results files with the new result files.

3. Run the tests again to verify that they pass.

These steps are implemented in script file UpdateInstallSolutions.csh (in directory Whisper/Utilities/Testing).

11.5 Computer Programs

11.5.1 Script File UpdateInstallSolutions.csh

11.5.1.1 Command Syntax

The syntax to execute UpdateInstallSolutions.csh is:

```
> UpdateInstallSolutions.csh
```

11.5.1.2 Operations

Script file UpdateInstallSolutions.csh (in directory Whisper/Utilities/Testing) performs the following:

1. Because this is a permanent change that can only be undone by a reinstall of Whisper, the user is requested to type confirm [LA-UR-14-23352; Sec. 6.3].
2. If the user enters “confirm”:
 - a. Change location to the testing directory (\$WHISPER_PATH/Testing).
 - b. Execute the script file RunInstallTests.csh (see Section 12 below) to run the installation tests.
 - c. If there are any differences between the test results and the reference solutions (i.e., file ‘Diff.dat’ exists):
 - 1) Update the reference solutions (files Test1.out, Test2.out, Reject2.dat, Test3.out, and cov.92235.dat) by:
 - a) Change the file system authority to allow the script to overwrite the reference file.
 - b) Copy the new test result to the reference file.
 - c) Change the file system authority to protect the reference file from user changes.
 - 2) Delete the installation test output files.
 - 3) Execute the script file RunInstallTests.csh to run the installation tests.
 - 4) Print the script results.

- a) If there are no differences between the test results and the reference solutions (i.e., file ‘Diff.dat’ does not exist), the update is complete.
- b) If there are any differences between the test results and the reference solutions (i.e., file ‘Diff.dat’ exists), the update failed.

11.5.1.3 V&V Activities

Script file UpdateInstallSolutions.csh can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	3 – 10
2.	12 – 70
2.a	17
2.b	18
2.c	20 – 64
2.c.1	24 – 43
2.c.2	45 – 51
2.c.3	53
2.c.4	54 – 64

11.5.1.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

12. Run Installation Tests

12.1 Output Data

If everything has been copied and installed correctly, the user gets a message indicating the all installation tests having passed. If failures occur, there will be difference files ‘Diffx.y.dat’ (here x is the test index and y is a file number within that test) that identify differences from reference files.

12.2 Input Data

No user input is required to run the installation files. The test input files are provided in directory Whisper/Testing/Installation. Directory Whisper/Testing/Installation also has the reference output files. The tests also rely on the data files (benchmarks, covariance, etc.) distributed with the Whisper program suite.

12.3 Algorithm Description

There is not an algorithm for running the installation tests, only a process which is described below.

12.4 Process Description

The following installation tests are performed [LA-UR-14-23352; Sec. 2.2]:

1. The first test checks the ability of Whisper to compute baseline USLs.

The test uses the benchmark suite provided with Whisper and excludes a majority of them. The benchmark information is obtained from the WHISPER BENCHMARK TOC environment variable, which tests this part of the installation. This test then computes the baseline USLs for a set of applications provided in the test. The output file ‘Test1.out’ is compared with a reference file.

2. The second test checks the benchmark rejection ability of Whisper.

A list of benchmarks is provided by the test; a user options file is also provided that changes the cutoff χ^2 value for acceptance from the default of 1.2 to 1.6. The test uses the iterative diagonal method to reject a series of benchmarks until the χ^2 of the suite falls below 1.6. The test compares the output file ‘Test2.out’ and the list of rejected benchmarks in ‘Reject2.out’.

3. The third test checks the GLLS nuclear covariance data adjustment capability of Whisper.

A list of benchmarks is provided by the test along with a set of benchmark correlations. The GLLS adjustment produces a new set of adjusted covariance data. The output file ‘Test3.out’ adjusted covariance file for U-235 is compared with the reference files.

If everything has been copied and installed correctly, the message indicating the all installation tests having passed will be displayed. If failures occur, there are difference files ‘Diffx.y.dat’ (here x is the test index and y is a file number within that test) that provide differences from reference files.

Note that if the benchmark suite distributed with Whisper is modified, these tests may not pass. In this case, advanced users may wish to replace the template files once they have checked that the results are otherwise correct so that this may be used as a check on any other potential changes to the system. A description of how to do this is given in Sec. 11 above.

12.5 Computer Programs

12.5.1 Script File Testing/Make

12.5.1.1 Command Syntax

Enter the ‘Testing’ directory and enter the command [LA-UR-14-23352; Sec. 2.2]:

```
> make install
```

This runs the installation tests, which typically takes about 10 minutes.

12.5.1.2 Operations

The ‘make install’ command executes the RunInstallTests.csh script file, i.e.,

```
> Installation/RunInstallTests.csh
```

12.5.1.3 V&V Activities

Script file Testing/Make can be verified and validated by a review of the script file. Lines 1 and 2 associate the ‘install’ argument with running the RunInstallTests.csh script file.

12.5.1.4 V&V Results

The review of script file Testing/Make has verified the command “make install” executes the script file RunInstallTests.csh.

12.5.2 Script File RunInstallTests.csh

12.5.2.1 Command Syntax

The syntax to execute RunInstallTests.csh is:

```
> Installation/RunInstallTests.csh
```

12.5.2.2 Operations

Script file RunInstallTests.csh performs the following:

1. Checks that the Whisper path environment variable is set.
2. Save the benchmark sensitivity data directory (first line in benchmark library file) in file ‘Header.tmp’.
3. Run test #1.
 - a. Save the differences with the reference file ‘Installation/Test1/Test1.out’ (other than lines with “Benchmark Library File”) to file ‘Diff1.1.dat’.

4. Run test #2.
 - a. Save the differences with the reference file ‘Installation/Test2/Test2.out’ to file ‘Diff2.1.dat’.
 - b. Save the differences with the reference file ‘Installation/Test2/Reject2.out’ to file ‘Diff2.2.dat’.
5. Run test #3.
 - a. Save the differences with the reference file ‘Installation/Test3/Test3.out’ to file ‘Diff3.1.dat’.
 - b. Save the differences with the reference file ‘Installation/Test3/cov.92235.dat’ to file ‘Diff3.2.dat’.
6. Merge the ‘Diff??.dat’ files into a single file ‘Diff.dat’.
7. Count the number of words in file ‘Diff.dat’.
8. If file ‘Diff.dat’ is empty, the installation tests have passed.
 - a. Delete the test output files.
9. If file ‘Diff.dat’ is not empty, the installation tests have failed.

12.5.2.3 V&V Activities

Script file RunInstallTests.csh can be verified and validated by a review of the script file. The following table cross references the operation steps (in the section above) to the script line numbers.

Operation Step	Script line numbers
1.	9 – 20
2.	23 – 28
3.	30 – 41
3.a	41
4.	43 – 62
4.a	61
4.b	62
5.	64 – 87
5.a	86
5.b	87
6.	89 – 92

Operation Step	Script line numbers
7.	96
8.	97 – 108
8.a	102 – 108
9.	109 - 111

12.5.2.4 V&V Results

The script lines for each operation step have been identified in the table above. The code review has determined that the script performs the listed operations.

13. Install and Uninstall Whisper Program Suite

The Whisper program suite includes a script file, Whisper/Install/InstallWhisper.csh, to install Whisper. This script is not individually reviewed here because all of the other validation and verification activities were performed after Whisper was installed.

The Whisper program suite also includes a script file, Whisper/Install/UninstallWhisper.csh, to uninstall Whisper. This script is not individually reviewed here because the intent of uninstalling a program is to terminate its use.

Also, the user can execute the install or uninstall script files with the Makefile in directory Whisper, i.e., command “make install” or “make uninstall”.

14. Compile Whisper Source Code

The Whisper/Source directory has a Makefile which contains the commands for compiling the Whisper source code. The command is:

```
> make all
```

This Makefile is not reviewed here because all V&V test activities were performed with the Whisper executable code.

15. References

- LA-CP-13-00634, Rev. 0, *MCNP6 User's Manual*, Version 1.0, May 2013
- LA-UR-10-06230, Rev 3, *An Expanded Criticality Validation Suite for MCNP*
- LA-UR-11-11271, *ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmark and Reactor Experiments*, (Nucl. Data Sheets, Vol. 112, page 2997, Dec. 2011)
- LA-UR-13-21822, Version 1, *Listing of Available ACE Data Tables*, 2013-06-05
- LA-UR-14-23202, *Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation*
- LA-UR-14-23352, *Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems*
- LA-UR-14-26436, *User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation*
- LA-UR-14-26558, *Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits*
- NCS-TECH-007-002, *Validation of MCNP5 on the Ganglion Cyst Computer Cluster with Various Cross Section Libraries*
- NCS-TECH-14-019, *Validation of MCNP6.1 on Moonlight for Plutonium and Uranium Systems*, December 16, 2014
- NCS-TECH-14-031, *Validation of MCNP6.1 on Luna for Generic Plutonium and Uranium Systems*, January 16, 2015
- ORNL/TM-2005/39, Version 6.1, *Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, June 2011
- Whisper Source Code Inspection Report*, R. F. Sartor and F. B. Brown, Los Alamos National Laboratory, LA-UR publication pending

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APPENDIX A – RunMCNPInputs.csh Modified Input File

The contents of file ‘pumetal_0.01_in’ in the Moonlight directory Whisper/ValidationFiles/vv/pumetal are:

```

1 Comparison Deck for Plutonium Validation - METAL SERIES
2 C
3 C A cylinder of Pu metal on a Stainless Steel 304 floor,
4 C with water "hands" reflection.
5 C
6 C Varying Parameters:
7 C H-to-D Ratio = 1
8 C Pu-240 Content = 0.01
9 C Mass Uranium = 6000 g
10 C
11 C Constant Parameters:
12 C GB Floor Thickness = 0.635 cm
13 C "Hand" thickness = 2.54 cm
14 C
15 C
16 C -----
17 C CELL CARDS
18 C -----
19 100 1 -19.86 -30 IMP:n=1
20 200 2 -1 +30 -40 IMP:n=1
21 300 3 -7.92 -10 +20 -99 IMP:n=1
22 400 0 -20 -99 IMP:n=1
23 500 0 +10 +40 -99 IMP:n=1
24 999 0 +99 IMP:n=0
25
26 C -----
27 C SURFACE CARDS
28 C -----
29 10 PZ 0.0
30 20 PZ -0.635
31 C
32 30 RCC 0.0 0.0 0.0 0.0 0.0 7.2726726771434 3.6363363385717
33 40 RCC 0.0 0.0 0.0 0.0 0.0 9.8126726771434 6.1763363385717

```

```
34 99 SO 50
35
36 C -----
37 C DATA CARDS
38 C -----
39 C
40 C
41 KCODE 30000 1.0 50 250
42 KSRC 0.0 0.0 3.6363363385717
43 C
44 C
45 C PLUTONIUM METAL: 19.86 g/cc
46 M1 94239.80c -0.99
47 94240.80c -0.01
48 C WATER: 1.00 g/cc
49 M2 1001.80c 0.6665933330
50 1002.80c 0.0000766671
51 8016.80c 0.33333
52 MT2 LWTR.20t
53 HWTR.20t
54 C SS 304: 7.92 g/cc
55 M3 24050.80c 0.0007573335
56 24052.80c 0.0146044227
57 24053.80c 0.0016560243
58 24054.80c 0.0004122195
59 25055.80c 0.00174
60 26054.80c 0.0034695920
61 26056.80c 0.0544651744
62 26057.80c 0.0012578384
63 26058.80c 0.0001673952
64 28058.80c 0.0052555367
65 28060.80c 0.0020244233
66 28061.80c 0.0000880003
67 28062.80c 0.0002805834
68 28064.80c 0.0000714563
69 MT3 FE56.22t
```

The contents of file 'pumetal_0.01_in' in the Moonlight directory Whisper/ValidationFiles/vv/pumetal/Calcs are:

```
1 Comparison Deck for Plutonium Validation - METAL SERIES
2 C
3 C A cylinder of Pu metal on a Stainless Steel 304 floor,
4 C with water "hands" reflection.
5 C
6 C Varying Parameters:
7 C H-to-D Ratio = 1
8 C Pu-240 Content = 0.01
9 C Mass Uranium = 6000 g
10 C
11 C Constant Parameters:
12 C GB Floor Thickness = 0.635 cm
13 C "Hand" thickness = 2.54 cm
14 C
15 C
16 C -----
17 C CELL CARDS
18 C -----
19 100 1 -19.86 -30 IMP:n=1
20 200 2 -1 +30 -40 IMP:n=1
21 300 3 -7.92 -10 +20 -99 IMP:n=1
22 400 0 -20 -99 IMP:n=1
23 500 0 +10 +40 -99 IMP:n=1
24 999 0 +99 IMP:n=0
25
26 C -----
27 C SURFACE CARDS
28 C -----
29 10 PZ 0.0
30 20 PZ -0.635
31 C
32 30 RCC 0.0 0.0 0.0 0.0 0.0 7.2726726771434 3.6363363385717
33 40 RCC 0.0 0.0 0.0 0.0 0.0 9.8126726771434 6.1763363385717
34 99 SO 50
35
```

```
36 C -----
37 C DATA CARDS
38 C -----
39 C
40 C
41 kcode 100000 1.0 100 600
42 kopts blocksize = 5
43 ksen1 xs
44     rxn = +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
45     erg = 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
46             4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
47             2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
48             4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
49             6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
50             3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
51             1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
52             6.4340e+00 8.1873e+00 2.0000e+01
53 prdmp j 9999999
54 KSRC 0.0 0.0 3.6363363385717
55 C
56 C
57 C PLUTONIUM METAL: 19.86 g/cc
58 M1    94239.80c -0.99
59        94240.80c -0.01
60 C WATER: 1.00 g/cc
61 M2    1001.80c  0.6665933330
62        1002.80c  0.0000766671
63        8016.80c  0.33333
64 MT2   LWTR.20t
65       HWTR.20t
66 C SS 304: 7.92 g/cc
67 M3    24050.80c 0.0007573335
68        24052.80c 0.0146044227
69        24053.80c 0.0016560243
70        24054.80c 0.0004122195
71        25055.80c 0.00174
72        26054.80c 0.0034695920
```

```
73      26056.80c  0.0544651744
74      26057.80c  0.0012578384
75      26058.80c  0.0001673952
76      28058.80c  0.0052555367
77      28060.80c  0.0020244233
78      28061.80c  0.0000880003
79      28062.80c  0.0002805834
80      28064.80c  0.0000714563
81 MT3    FE56.22t
```

Comparing these two files, shows:

1. Lines 1 thru 40 are identical.
2. Line 41 (KCODE 30000 1.0 50 250) is replaced with:

```
41 kcode 100000 1.0 100 600
42 kopts blocksize = 5
43 ksen1 xs
44     rxn = +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
45     erg = 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
46             4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
47             2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
48             4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
49             6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
50             3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
51             1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
52             6.4340e+00 8.1873e+00 2.0000e+01
53 prdmp j 9999999
```

3. The rest of the original file (lines 42 thru 69) become lines 54 thru 81 in the modified file.

APPENDIX B – KeffSenList.toc File

The following listing is from file ‘KeffSenList.toc’ in the Moonlight directory Whisper/ValidationFiles/vv/pumetal.

```
1 /panfs/scratch/avol3/akersting/vv/pumetal/KeffSenLib/
2   pumetal_0.01_in           0.0000  0.0000  0.92757  0.00009
3   pumetal_0.02_in           0.0000  0.0000  0.92475  0.00009
4   pumetal_0.03_in           0.0000  0.0000  0.92247  0.00009
5   pumetal_0.04_in           0.0000  0.0000  0.92007  0.00009
6   pumetal_0.05_in           0.0000  0.0000  0.91769  0.00009
7   pumetal_0.06_in           0.0000  0.0000  0.91520  0.00009
8   pumetal_0.07_in           0.0000  0.0000  0.91282  0.00009
9   pumetal_0.08_in           0.0000  0.0000  0.91052  0.00009
10  pumetal_0.09_in           0.0000  0.0000  0.90812  0.00009
11  pumetal_0.11_in           0.0000  0.0000  0.90332  0.00010
12  pumetal_0.12_in           0.0000  0.0000  0.90111  0.00009
13  pumetal_0.13_in           0.0000  0.0000  0.89864  0.00009
14  pumetal_0.14_in           0.0000  0.0000  0.89619  0.00009
15  pumetal_0.15_in           0.0000  0.0000  0.89367  0.00009
16  pumetal_0.16_in           0.0000  0.0000  0.89145  0.00009
17  pumetal_0.17_in           0.0000  0.0000  0.88893  0.00009
18  pumetal_0.18_in           0.0000  0.0000  0.88664  0.00009
19  pumetal_0.19_in           0.0000  0.0000  0.88416  0.00009
20  pumetal_0.1_in            0.0000  0.0000  0.90582  0.00009
21  pumetal_0.2_in            0.0000  0.0000  0.88164  0.00009
22  pumetal_1e-06_in          0.0000  0.0000  0.93061  0.00009
```

Lines 4747 to 4766 of file ‘pumetal_0.01_ino’ in directory Whisper/ValidationFiles/vv/pumetal/Calcs are:

```
the final estimated combined collision/absorption/track-length keff = 0.92757 with an estimated standard deviation of 0.00009
the estimated 68, 95, & 99 percent keff confidence intervals are 0.92748 to 0.92766, 0.92738 to 0.92775, and 0.92733 to 0.92781
the final combined (col/abs/tl) prompt removal lifetime = 3.3409E-06 seconds with an estimated standard deviation of 2.9728E-09
the average neutron energy causing fission = 1.7529E+00 mev
the energy corresponding to the average neutron lethargy causing fission = 5.3869E-01 mev
the percentages of fissions caused by neutrons in the thermal, intermediate, and fast neutron ranges are:
    (<0.625 ev):   2.11%           (0.625 ev - 100 kev):   7.91%           (>100 kev):   89.99%
the average fission neutrons produced per neutron absorbed (capture + fission) in all cells with fission = 2.9265E+00
the average fission neutrons produced per neutron absorbed (capture + fission) in all the geometry cells = 2.8731E+00
the average number of neutrons produced per fission = 3.133
```

A comparison of the two files shows the MCNP6 results, the application k_{eff} and uncertainty values on line 4749, are correctly copied to the file ‘KeffSenList.toc’ (line 2).

APPENDIX C – ORNL and Whisper Energy Groups

The first 15 lines of ‘Whisper/CovarianceData/SCALE6.1/Native/ORNL_SCALE6.1.cov’ are:

```

1 0v v7rec ornl-10/2008      1
2 1d    44    44    0     2   2589   2558      3
3 2d coverx file for v7
4 3d  2.0000E+07  8.1873E+06  6.4340E+06  4.8000E+06  3.0000E+06
5   2.4790E+06  2.3540E+06  1.8500E+06  1.4000E+06  9.0000E+05  4.0000E+05
6   1.0000E+05  2.5000E+04  1.7000E+04  3.0000E+03  5.5000E+02  1.0000E+02
7   3.0000E+01  1.0000E+01  8.1000E+00  6.0000E+00  4.7500E+00  3.0000E+00
8   1.7700E+00  1.0000E+00  6.2500E-01  4.0000E-01  3.7500E-01  3.5000E-01
9   3.2500E-01  2.7500E-01  2.5000E-01  2.2500E-01  2.0000E-01  1.5000E-01
10  1.0000E-01  7.0000E-02  5.0000E-02  4.0000E-02  3.0000E-02  2.5300E-02
11  1.0000E-02  7.5000E-03  3.0000E-03  1.0000E-05
12 5d    1801      2      4   1801     102      4   1801      1      4   1802      1      4
13   1802      2      4   1802     102      4   1802      16      4   1003      1      4
14   1003     16      4   1003      2      4   2003      1      4   2003      2      4
15   2003     102      4   2003     103      4   2003     104      4   2004      1      4

```

For a COVERX file, the “3d” data block is the neutron group boundaries in units of eV in decreasing order [ORNL/TM-2005/39; Table M18.A.8].

The ‘SCALE44ErgGrid.dat’ file distributed with Whisper is:

```

1 rxn = +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
2 erg = 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
3   4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
4   2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
5   4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
6   6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
7   3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
8   1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
9   6.4340e+00 8.1873e+00 2.0000e+01

```

For the MCNP6 KSEN card, the energy bins (erg values) are in ascending order [LA-CP-13-00634; Table 3-103 in Sec. 3.3.5.23]. MCNP6 uses energy units of MeV [LA-CP-13-00634; Sec. 2].

The energy groups in Whisper (module ParametersMod) are:

```
32      ! SCALE6.1 44-group energy bin structure
33      real(8), parameter :: EBins(1:NErg+1) = &
34      [ 1.0000e-11, 3.0000e-09, 7.5000e-09, 1.0000e-08, 2.5300e-08, 3.0000e-08, &
35      & 4.0000e-08, 5.0000e-08, 7.0000e-08, 1.0000e-07, 1.5000e-07, 2.0000e-07, &
36      & 2.2500e-07, 2.5000e-07, 2.7500e-07, 3.2500e-07, 3.5000e-07, 3.7500e-07, &
37      & 4.0000e-07, 6.2500e-07, 1.0000e-06, 1.7700e-06, 3.0000e-06, 4.7500e-06, &
38      & 6.0000e-06, 8.1000e-06, 1.0000e-05, 3.0000e-05, 1.0000e-04, 5.5000e-04, &
39      & 3.0000e-03, 1.7000e-02, 2.5000e-02, 1.0000e-01, 4.0000e-01, 9.0000e-01, &
40      & 1.4000e+00, 1.8500e+00, 2.3540e+00, 2.4790e+00, 3.0000e+00, 4.8000e+00, &
41      & 6.4340e+00, 8.1873e+00, 2.0000e+01 ]
```

After accounting for any differences in units and ordering, the three blocks of energy boundaries are identical.

References

- LA-CP-13-00634, Rev. 0, *MCNP6 User's Manual*, May 2013
- ORNL/TM-2005/39, Version 6.1, *Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, June 2011

APPENDIX D – Reaction Numbers

The ‘SCALE44ErgGrid.dat’ file distributed with Whisper is:

```

1      rxn = +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
2      erg = 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
3          4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
4          2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
5          4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
6          6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
7          3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
8          1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
9          6.4340e+00 8.1873e+00 2.0000e+01

```

For the MCNP6 KSEN card, the MT Numbers and/or the Special Reaction Numbers in Table 3-104 of LA-CP-13-00634, Sec. 3.3.5.23, can be used for the reaction (rxn) values.

The reaction numbers in Whisper (module ParametersMod) are:

```

43      ! list of relevant MT reaction numbers
44      integer, parameter, public :: NumRelevantMTs = 12
45      integer, parameter, public :: RelevantMT(NumRelevantMTs) = &
46      & [ 2, 4, 18, 16, 102, 103, 104, 105, 106, 107, 452, 1018 ]

```

The RelevantMT numbers in Whisper are used with the covariance data which originated from SCALE 6.1. The MT reaction types are described in Section M4.B of ORNL/TM-2005/39. Values from 1 to 999 are ENDF reaction types. MT numbers greater than 999 are additional SCALE-specific identifiers.

The following table compares the MCNP6 reaction (rxn) number against the RelevantMT numbers in Whisper. Although there are apparent differences between some values, the rxn and RelevantMT values correspond to the same reaction data.

Seq. #	MCNP6 RXN Value	Description [LA-CP-13-00634]	Whisper MT Value	Description [ORNL/TM-2005/39]
1.	2	MT for Elastic.	2	(z,z ₀); Elastic scattering cross section for incident particles.

Seq. #	MCNP6 RXN Value	Description [LA-CP-13-00634]	Whisper MT Value	Description [ORNL/TM-2005/39]
2.	4	MT for Total Inelastic.	4	(z,n); Production of one neutron in the exit channel. For incident neutrons, this is the total inelastic scattering [http://t2.lanl.gov/nis/endf/mts.html].
3.	-6	RN for Total Fission; equivalent to MT of 18.	18	(z,fission)
4.	16	MT for (n,2n).	16	(z,2n); Production of two neutrons.
5.	102	MT for (n, γ).	102	(z, γ); Radiative capture.
6.	103	MT for (n,p).	103	(z,p); Production of a proton.
7.	104	MT for (n,d).	104	(z,d); Production of a deuteron.
8.	105	MT for (n,t).	105	(z,t); Production of a triton.
9.	106	MT for (n, ${}^3\text{He}$).	106	(z, ${}^3\text{He}$); Production of a ${}^3\text{He}$.
10.	107	MT for (n, α).	107	(z, α); Production of an alpha particle.
11.	-7	RN for total fission v; equivalent to MT of 452.	452	\bar{v}_T , average total number of neutrons released per fission
12.	-1018	RN for total fission chi.	1018	Fission spectrum.

Note: The Whisper code assumes the sensitivity data is in the sequential order listed above.

References

- <http://t2.lanl.gov/nis/endf/mts.html>, ENDF MT Values, T-2 Nuclear Information Service, 23 January 1998
- LA-CP-13-00634, Rev. 0, MCNP6 User's Manual, May 2013
- ORNL/TM-2005/39, Version 6.1, Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, June 2011

APPENDIX E – File BenchCorrel.dat

The correlation data in the file ‘Benchmark/Correlations/BenchCorrel.dat’ is:

1	heu-met-fast-008-001.i	heu-met-fast-011-001.i	0.2100
2	heu-met-fast-020-002.i	heu-met-fast-031-001.i	0.4600
3	heu-met-fast-067-001.i	heu-met-fast-067-002.i	0.9600
4	heu-sol-therm-001-001.i	heu-sol-therm-001-002.i	0.4700
5	heu-sol-therm-001-001.i	heu-sol-therm-001-003.i	0.4600
6	heu-sol-therm-001-001.i	heu-sol-therm-001-004.i	0.4400
7	heu-sol-therm-001-001.i	heu-sol-therm-001-005.i	0.4200
8	heu-sol-therm-001-001.i	heu-sol-therm-001-006.i	0.4200
9	heu-sol-therm-001-001.i	heu-sol-therm-001-007.i	0.4600
10	heu-sol-therm-001-001.i	heu-sol-therm-001-008.i	0.5700
11	heu-sol-therm-001-001.i	heu-sol-therm-001-009.i	0.4400
12	heu-sol-therm-001-001.i	heu-sol-therm-001-010.i	0.4400
13	heu-sol-therm-001-002.i	heu-sol-therm-001-003.i	0.4200
14	heu-sol-therm-001-002.i	heu-sol-therm-001-004.i	0.5800
15	heu-sol-therm-001-002.i	heu-sol-therm-001-005.i	0.4200
16	heu-sol-therm-001-002.i	heu-sol-therm-001-006.i	0.4200
17	heu-sol-therm-001-002.i	heu-sol-therm-001-007.i	0.4100
18	heu-sol-therm-001-002.i	heu-sol-therm-001-008.i	0.4400
19	heu-sol-therm-001-002.i	heu-sol-therm-001-009.i	0.5800
20	heu-sol-therm-001-002.i	heu-sol-therm-001-010.i	0.4600
21	heu-sol-therm-001-003.i	heu-sol-therm-001-004.i	0.4600
22	heu-sol-therm-001-003.i	heu-sol-therm-001-005.i	0.4300
23	heu-sol-therm-001-003.i	heu-sol-therm-001-006.i	0.4300
24	heu-sol-therm-001-003.i	heu-sol-therm-001-007.i	0.4600
25	heu-sol-therm-001-003.i	heu-sol-therm-001-008.i	0.4600
26	heu-sol-therm-001-003.i	heu-sol-therm-001-009.i	0.4200
27	heu-sol-therm-001-003.i	heu-sol-therm-001-010.i	0.4300
28	heu-sol-therm-001-004.i	heu-sol-therm-001-005.i	0.4200
29	heu-sol-therm-001-004.i	heu-sol-therm-001-006.i	0.4200
30	heu-sol-therm-001-004.i	heu-sol-therm-001-007.i	0.4200
31	heu-sol-therm-001-004.i	heu-sol-therm-001-008.i	0.4400
32	heu-sol-therm-001-004.i	heu-sol-therm-001-009.i	0.7700
33	heu-sol-therm-001-004.i	heu-sol-therm-001-010.i	0.4600

34	heu-sol-therm-001-005.i	heu-sol-therm-001-006.i	0.5400
35	heu-sol-therm-001-005.i	heu-sol-therm-001-007.i	0.4800
36	heu-sol-therm-001-005.i	heu-sol-therm-001-008.i	0.4700
37	heu-sol-therm-001-005.i	heu-sol-therm-001-009.i	0.4600
38	heu-sol-therm-001-005.i	heu-sol-therm-001-010.i	0.4800
39	heu-sol-therm-001-006.i	heu-sol-therm-001-007.i	0.4800
40	heu-sol-therm-001-006.i	heu-sol-therm-001-008.i	0.4700
41	heu-sol-therm-001-006.i	heu-sol-therm-001-009.i	0.4600
42	heu-sol-therm-001-006.i	heu-sol-therm-001-010.i	0.4800
43	heu-sol-therm-001-007.i	heu-sol-therm-001-008.i	0.5100
44	heu-sol-therm-001-007.i	heu-sol-therm-001-009.i	0.4500
45	heu-sol-therm-001-007.i	heu-sol-therm-001-010.i	0.4300
46	heu-sol-therm-001-008.i	heu-sol-therm-001-009.i	0.4800
47	heu-sol-therm-001-008.i	heu-sol-therm-001-010.i	0.4400
48	heu-sol-therm-001-009.i	heu-sol-therm-001-010.i	0.4600
49	heu-sol-therm-009-001.i	heu-sol-therm-009-002.i	0.6100
50	heu-sol-therm-009-001.i	heu-sol-therm-009-003.i	0.5800
51	heu-sol-therm-009-001.i	heu-sol-therm-010-001.i	0.1800
52	heu-sol-therm-009-001.i	heu-sol-therm-011-001.i	0.2300
53	heu-sol-therm-009-001.i	heu-sol-therm-011-002.i	0.2300
54	heu-sol-therm-009-001.i	heu-sol-therm-012-001.i	0.2900
55	heu-sol-therm-009-001.i	heu-sol-therm-043-001.i	0.1300
56	heu-sol-therm-009-001.i	heu-sol-therm-043-002.i	0.2900
57	heu-sol-therm-009-001.i	heu-sol-therm-043-003.i	0.2900
58	heu-sol-therm-009-002.i	heu-sol-therm-009-003.i	0.6000
59	heu-sol-therm-009-002.i	heu-sol-therm-010-001.i	0.1700
60	heu-sol-therm-009-002.i	heu-sol-therm-011-001.i	0.2000
61	heu-sol-therm-009-002.i	heu-sol-therm-011-002.i	0.2000
62	heu-sol-therm-009-002.i	heu-sol-therm-012-001.i	0.2500
63	heu-sol-therm-009-002.i	heu-sol-therm-043-001.i	0.1400
64	heu-sol-therm-009-002.i	heu-sol-therm-043-002.i	0.2500
65	heu-sol-therm-009-002.i	heu-sol-therm-043-003.i	0.2600
66	heu-sol-therm-009-003.i	heu-sol-therm-010-001.i	0.1500
67	heu-sol-therm-009-003.i	heu-sol-therm-011-001.i	0.1600
68	heu-sol-therm-009-003.i	heu-sol-therm-011-002.i	0.1600
69	heu-sol-therm-009-003.i	heu-sol-therm-012-001.i	0.1800
70	heu-sol-therm-009-003.i	heu-sol-therm-043-001.i	0.1200

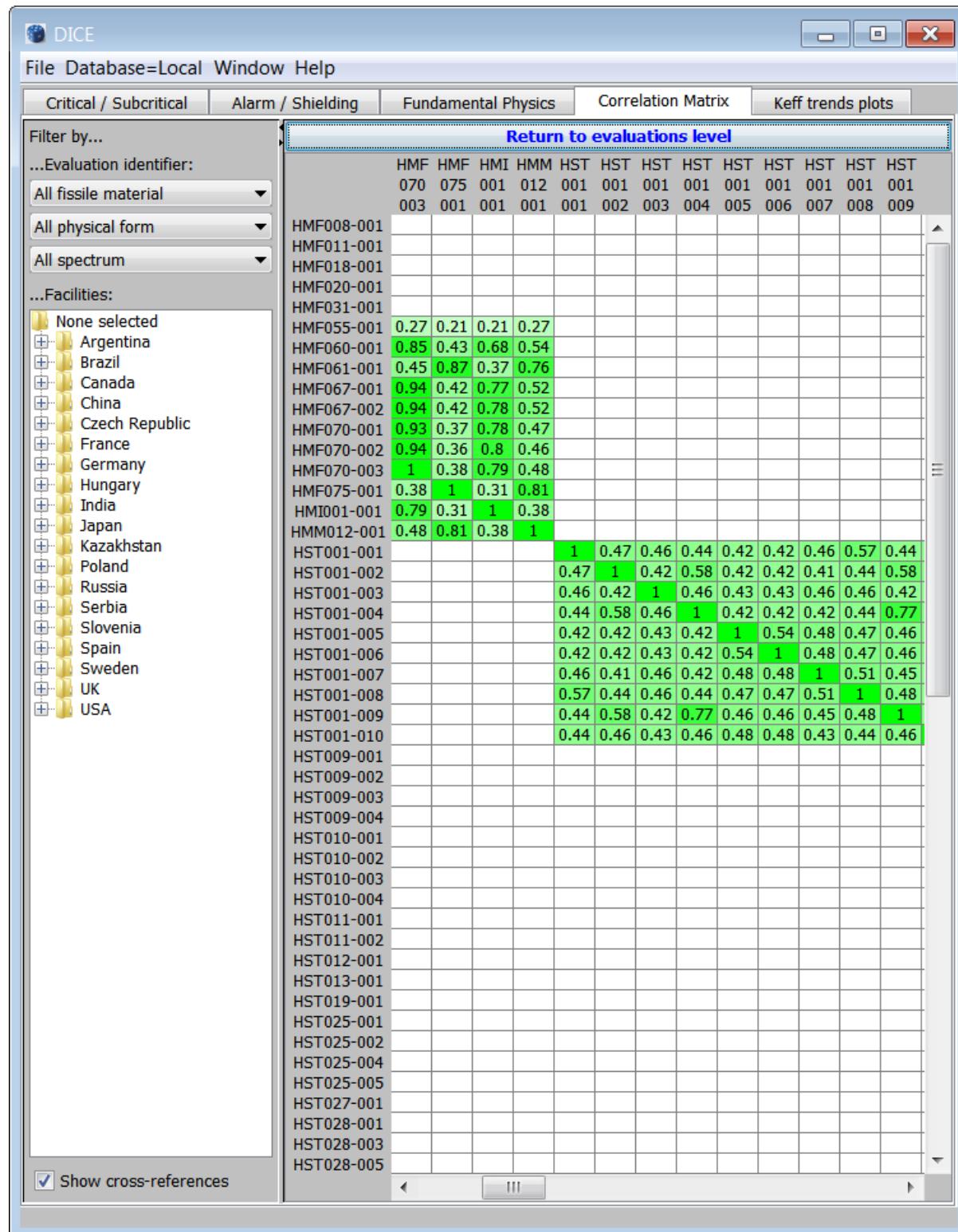
71	heu-sol-therm-009-003.i	heu-sol-therm-043-002.i	0.1900
72	heu-sol-therm-009-003.i	heu-sol-therm-043-003.i	0.1900
73	heu-sol-therm-010-001.i	heu-sol-therm-011-001.i	0.1100
74	heu-sol-therm-010-001.i	heu-sol-therm-011-002.i	0.1100
75	heu-sol-therm-010-001.i	heu-sol-therm-012-001.i	0.1200
76	heu-sol-therm-010-001.i	heu-sol-therm-043-001.i	0.0800
77	heu-sol-therm-010-001.i	heu-sol-therm-043-002.i	0.1200
78	heu-sol-therm-010-001.i	heu-sol-therm-043-003.i	0.1200
79	heu-sol-therm-011-001.i	heu-sol-therm-011-002.i	0.5300
80	heu-sol-therm-011-001.i	heu-sol-therm-012-001.i	0.2400
81	heu-sol-therm-011-001.i	heu-sol-therm-043-001.i	0.4700
82	heu-sol-therm-011-001.i	heu-sol-therm-043-002.i	0.2400
83	heu-sol-therm-011-001.i	heu-sol-therm-043-003.i	0.2500
84	heu-sol-therm-011-002.i	heu-sol-therm-012-001.i	0.2400
85	heu-sol-therm-011-002.i	heu-sol-therm-043-001.i	0.4700
86	heu-sol-therm-011-002.i	heu-sol-therm-043-002.i	0.2400
87	heu-sol-therm-011-002.i	heu-sol-therm-043-003.i	0.2500
88	heu-sol-therm-012-001.i	heu-sol-therm-043-001.i	0.0500
89	heu-sol-therm-012-001.i	heu-sol-therm-043-002.i	0.4700
90	heu-sol-therm-012-001.i	heu-sol-therm-043-003.i	0.3600
91	heu-sol-therm-013-001.i	heu-sol-therm-032-001.i	0.4100
92	heu-sol-therm-013-001.i	heu-sol-therm-042-001.i	0.2900
93	heu-sol-therm-013-001.i	heu-sol-therm-042-002.i	0.3100
94	heu-sol-therm-013-001.i	heu-sol-therm-042-003.i	0.3800
95	heu-sol-therm-013-001.i	heu-sol-therm-042-004.i	0.3600
96	heu-sol-therm-013-001.i	heu-sol-therm-042-005.i	0.3700
97	heu-sol-therm-013-001.i	heu-sol-therm-042-006.i	0.3500
98	heu-sol-therm-013-001.i	heu-sol-therm-042-007.i	0.3600
99	heu-sol-therm-013-001.i	heu-sol-therm-043-001.i	0.3500
100	heu-sol-therm-013-001.i	heu-sol-therm-043-002.i	0.1100
101	heu-sol-therm-019-001.i	heu-sol-therm-025-001.i	0.4500
102	heu-sol-therm-019-001.i	heu-sol-therm-025-002.i	0.4500
103	heu-sol-therm-019-001.i	heu-sol-therm-025-004.i	0.4300
104	heu-sol-therm-019-001.i	heu-sol-therm-025-005.i	0.4100
105	heu-sol-therm-025-001.i	heu-sol-therm-025-002.i	0.7300
106	heu-sol-therm-025-001.i	heu-sol-therm-025-004.i	0.7200
107	heu-sol-therm-025-001.i	heu-sol-therm-025-005.i	0.6200

108	heu-sol-therm-025-002.i	heu-sol-therm-025-004.i	0.7200
109	heu-sol-therm-025-002.i	heu-sol-therm-025-005.i	0.6200
110	heu-sol-therm-025-004.i	heu-sol-therm-025-005.i	0.6200
111	heu-sol-therm-042-001.i	heu-sol-therm-042-002.i	0.4600
112	heu-sol-therm-042-001.i	heu-sol-therm-042-003.i	0.3800
113	heu-sol-therm-042-001.i	heu-sol-therm-042-004.i	0.3600
114	heu-sol-therm-042-001.i	heu-sol-therm-042-005.i	0.3500
115	heu-sol-therm-042-001.i	heu-sol-therm-042-006.i	0.4200
116	heu-sol-therm-042-001.i	heu-sol-therm-042-007.i	0.3700
117	heu-sol-therm-042-001.i	heu-sol-therm-042-008.i	0.3500
118	heu-sol-therm-042-002.i	heu-sol-therm-042-003.i	0.4000
119	heu-sol-therm-042-002.i	heu-sol-therm-042-004.i	0.3900
120	heu-sol-therm-042-002.i	heu-sol-therm-042-005.i	0.3800
121	heu-sol-therm-042-002.i	heu-sol-therm-042-006.i	0.4400
122	heu-sol-therm-042-002.i	heu-sol-therm-042-007.i	0.4000
123	heu-sol-therm-042-002.i	heu-sol-therm-042-008.i	0.3700
124	heu-sol-therm-042-003.i	heu-sol-therm-042-004.i	0.4600
125	heu-sol-therm-042-003.i	heu-sol-therm-042-005.i	0.4600
126	heu-sol-therm-042-003.i	heu-sol-therm-042-006.i	0.4400
127	heu-sol-therm-042-003.i	heu-sol-therm-042-007.i	0.4500
128	heu-sol-therm-042-003.i	heu-sol-therm-042-008.i	0.4500
129	heu-sol-therm-042-004.i	heu-sol-therm-042-005.i	0.4800
130	heu-sol-therm-042-004.i	heu-sol-therm-042-006.i	0.4700
131	heu-sol-therm-042-004.i	heu-sol-therm-042-007.i	0.4800
132	heu-sol-therm-042-004.i	heu-sol-therm-042-008.i	0.4800
133	heu-sol-therm-042-005.i	heu-sol-therm-042-006.i	0.4700
134	heu-sol-therm-042-005.i	heu-sol-therm-042-007.i	0.4800
135	heu-sol-therm-042-005.i	heu-sol-therm-042-008.i	0.4800
136	heu-sol-therm-042-006.i	heu-sol-therm-042-007.i	0.5100
137	heu-sol-therm-042-006.i	heu-sol-therm-042-008.i	0.5000
138	heu-sol-therm-042-007.i	heu-sol-therm-042-008.i	0.5200
139	heu-sol-therm-043-001.i	heu-sol-therm-043-002.i	0.0600
140	heu-sol-therm-043-001.i	heu-sol-therm-043-003.i	0.0500
141	heu-sol-therm-043-002.i	heu-sol-therm-043-003.i	0.3500
142	mix-comp-fast-001-001.i	mix-comp-fast-002-001.i	0.6600

APPENDIX F – DICE Correlation Matrix

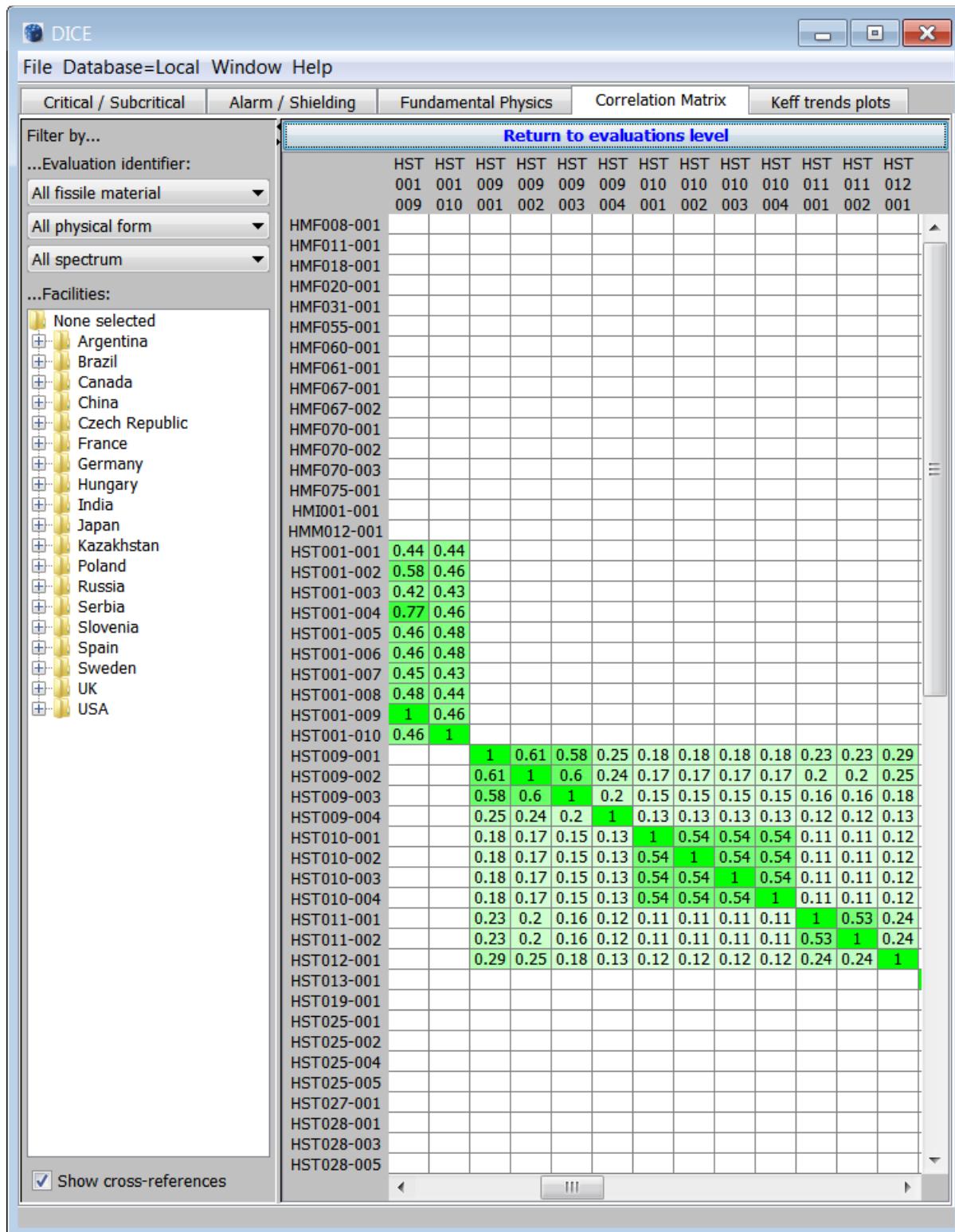
The following screen shots display the correlation matrix in the September 2013 Ed. of DICE.

The matrix is in two rows of eight figures. The screen shots overlap each other by one column or row to illustrate continuity. The matrix uses abbreviations of the ICSBEP benchmark names. For example, HEU-MET-FAST-008-001 is abbreviated to HMF008-001.



The screenshot shows the DICE software interface with the title bar "DICE". The menu bar includes "File", "Database=Local", "Window", "Help". The toolbar has buttons for "Critical / Subcritical", "Alarm / Shielding", "Fundamental Physics", "Correlation Matrix" (which is selected), and "Keff trends plots". A filter panel on the left contains dropdowns for "Evaluation identifier" (set to "All fissile material") and "Facilities" (a tree view showing countries: Argentina, Brazil, Canada, China, Czech Republic, France, Germany, Hungary, India, Japan, Kazakhstan, Poland, Russia, Serbia, Slovenia, Spain, Sweden, UK, USA). A checkbox "Show cross-references" is checked at the bottom of the filter panel. The main area displays a correlation matrix titled "Return to evaluations level". The columns and rows are labeled with benchmark names: HMF, HMF, HMI, HMM, HST, HST. The first row contains values: 070, 075, 001, 012, 001, 001, 001, 001, 001, 001, 001, 001, 001, 001, 001, 001, 001. The first column contains values: 003, 001, 001, 001, 001, 002, 003, 004, 005, 006, 007, 008, 009. The matrix itself contains numerical values representing correlations between pairs of benchmarks. The matrix is mostly empty, with non-zero values appearing in the first few rows and columns.

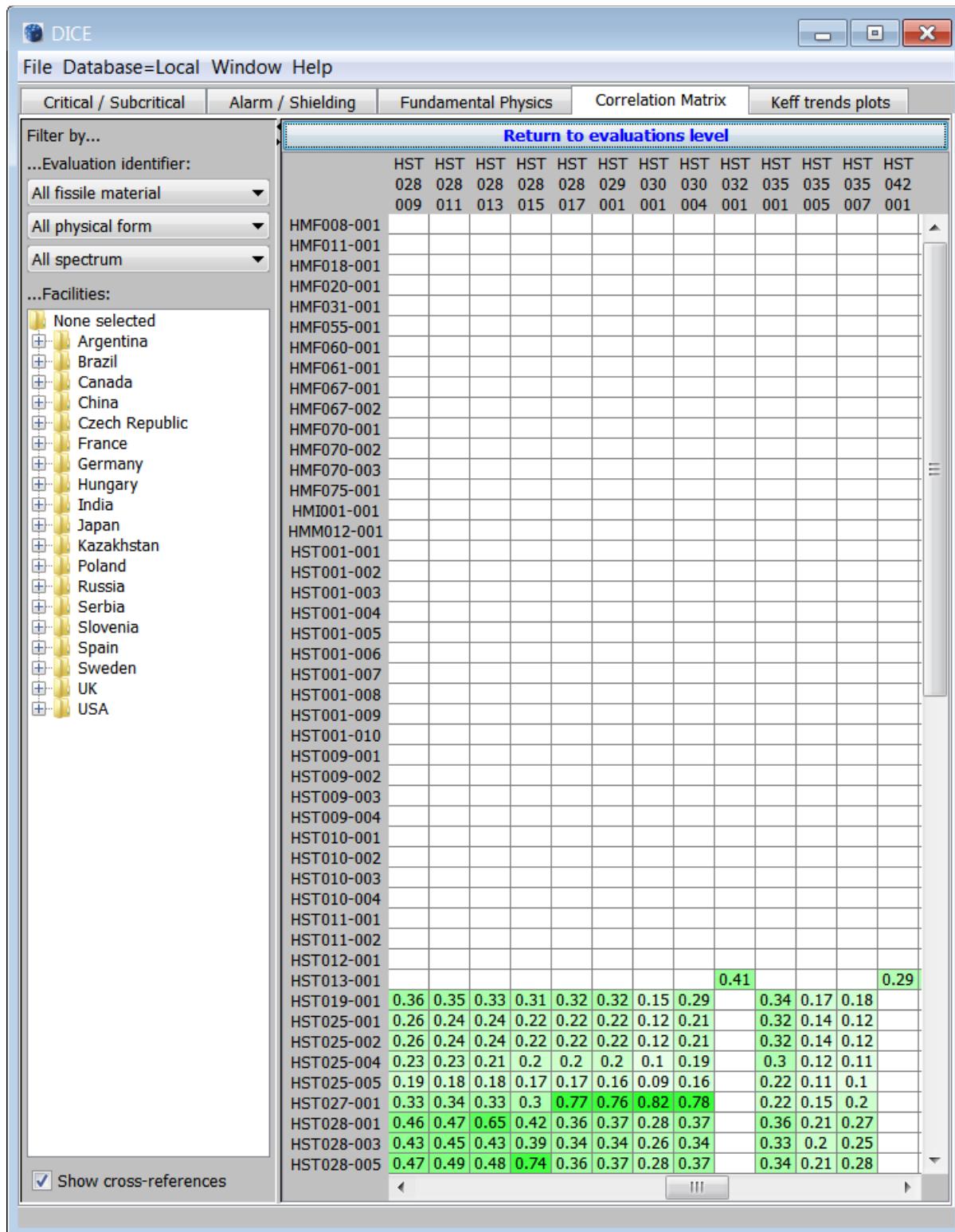
Return to evaluations level															
HMF	HMF	HMI	HMM	HST	HST	HST									
070	075	001	012	001	001	001	001	001	001	001	001	001	001	001	001
003	001	001	001	001	002	003	004	005	006	007	008	009			
HMF008-001															
HMF011-001															
HMF018-001															
HMF020-001															
HMF031-001															
HMF055-001	0.27	0.21	0.21	0.27											
HMF060-001	0.85	0.43	0.68	0.54											
HMF061-001	0.45	0.87	0.37	0.76											
HMF067-001	0.94	0.42	0.77	0.52											
HMF067-002	0.94	0.42	0.78	0.52											
HMF070-001	0.93	0.37	0.78	0.47											
HMF070-002	0.94	0.36	0.8	0.46											
HMF070-003	1	0.38	0.79	0.48											
HMF075-001	0.38	1	0.31	0.81											
HMI001-001	0.79	0.31	1	0.38											
HMM012-001	0.48	0.81	0.38	1											
HST001-001					1	0.47	0.46	0.44	0.42	0.42	0.46	0.57	0.44		
HST001-002					0.47	1	0.42	0.58	0.42	0.42	0.41	0.44	0.58		
HST001-003					0.46	0.42	1	0.46	0.43	0.43	0.46	0.46	0.42		
HST001-004					0.44	0.58	0.46	1	0.42	0.42	0.42	0.44	0.77		
HST001-005					0.42	0.42	0.43	0.42	1	0.54	0.48	0.47	0.46		
HST001-006					0.42	0.42	0.43	0.42	0.54	1	0.48	0.47	0.46		
HST001-007					0.46	0.41	0.46	0.42	0.48	0.48	1	0.51	0.45		
HST001-008					0.57	0.44	0.46	0.44	0.47	0.47	0.51	1	0.48		
HST001-009					0.44	0.58	0.42	0.77	0.46	0.46	0.45	0.48	1		
HST001-010					0.44	0.46	0.43	0.46	0.48	0.48	0.43	0.44	0.46		
HST009-001															
HST009-002															
HST009-003															
HST009-004															
HST010-001															
HST010-002															
HST010-003															
HST010-004															
HST011-001															
HST011-002															
HST012-001															
HST013-001															
HST019-001															
HST025-001															
HST025-002															
HST025-004															
HST025-005															
HST027-001															
HST028-001															
HST028-003															
HST028-005															



DICE

File Database=Local Window Help

	Critical / Subcritical	Alarm / Shielding	Fundamental Physics	Correlation Matrix	Keff trends plots
Filter by...					
...Evaluation identifier:					
All fissile material	HST	HST	HST	HST	HST
	012	013	019	025	025
	001	001	001	002	004
All physical form	025	025	025	025	027
All spectrum	005	005	001	001	003
...Facilities:	028	028	003	005	007
None selected	028	028	028	028	028
Argentina	009				
Brazil					
Canada					
China					
Czech Republic					
France					
Germany					
Hungary					
India					
Japan					
Kazakhstan					
Poland					
Russia					
Serbia					
Slovenia					
Spain					
Sweden					
UK					
USA					
<input checked="" type="checkbox"/> Show cross-references					
Return to evaluations level					
HST008-001	0.29	0.25	0.18	0.13	0.12
HST011-001	0.25	0.22	0.18	0.13	0.12
HST018-001	0.18	0.22	0.20	0.15	0.14
HST020-001	0.13	0.18	0.15	0.10	0.10
HST031-001	0.12	0.18	0.15	0.10	0.10
HMF008-001	0.29	0.25	0.18	0.13	0.12
HMF011-001	0.25	0.22	0.18	0.13	0.12
HMF018-001	0.18	0.22	0.20	0.15	0.14
HMF020-001	0.13	0.18	0.15	0.10	0.10
HMF031-001	0.12	0.18	0.15	0.10	0.10
HMF055-001	0.29	0.25	0.18	0.13	0.12
HMF060-001	0.25	0.22	0.18	0.13	0.12
HMF061-001	0.18	0.22	0.20	0.15	0.14
HMF067-001	0.13	0.18	0.15	0.10	0.10
HMF067-002	0.12	0.18	0.15	0.10	0.10
HMF070-001	0.29	0.25	0.18	0.13	0.12
HMF070-002	0.25	0.22	0.18	0.13	0.12
HMF070-003	0.18	0.22	0.20	0.15	0.14
HMF075-001	0.13	0.18	0.15	0.10	0.10
HMI001-001	0.12	0.18	0.15	0.10	0.10
HMM012-001	0.29	0.25	0.18	0.13	0.12
HST001-001	0.25	0.22	0.18	0.13	0.12
HST001-002	0.18	0.22	0.20	0.15	0.14
HST001-003	0.13	0.18	0.15	0.10	0.10
HST001-004	0.12	0.18	0.15	0.10	0.10
HST001-005	0.29	0.25	0.18	0.13	0.12
HST001-006	0.25	0.22	0.18	0.13	0.12
HST001-007	0.18	0.22	0.20	0.15	0.14
HST001-008	0.13	0.18	0.15	0.10	0.10
HST001-009	0.12	0.18	0.15	0.10	0.10
HST001-010	0.29	0.25	0.18	0.13	0.12
HST009-001	0.25	0.22	0.18	0.13	0.12
HST009-002	0.18	0.22	0.20	0.15	0.14
HST009-003	0.13	0.18	0.15	0.10	0.10
HST010-001	0.12	0.18	0.15	0.10	0.10
HST010-002	0.29	0.25	0.18	0.13	0.12
HST010-003	0.25	0.22	0.18	0.13	0.12
HST010-004	0.18	0.22	0.20	0.15	0.14
HST011-001	0.24	0.22	0.18	0.13	0.12
HST011-002	0.24	0.22	0.18	0.13	0.12
HST012-001	1	1	0.29	0.25	0.18
HST013-001	1	1	0.25	0.22	0.18
HST019-001	0.45	0.45	0.45	0.43	0.41
HST025-001	0.45	1	0.73	0.72	0.62
HST025-002	0.45	0.73	1	0.72	0.62
HST025-004	0.43	0.72	0.72	1	0.62
HST025-005	0.41	0.62	0.62	0.62	1
HST027-001	0.13	0.09	0.09	0.09	0.08
HST028-001	0.26	0.2	0.2	0.19	0.15
HST028-003	0.23	0.19	0.19	0.17	0.14
HST028-005	0.2	0.16	0.16	0.14	0.12



DICE

File Database=Local Window Help

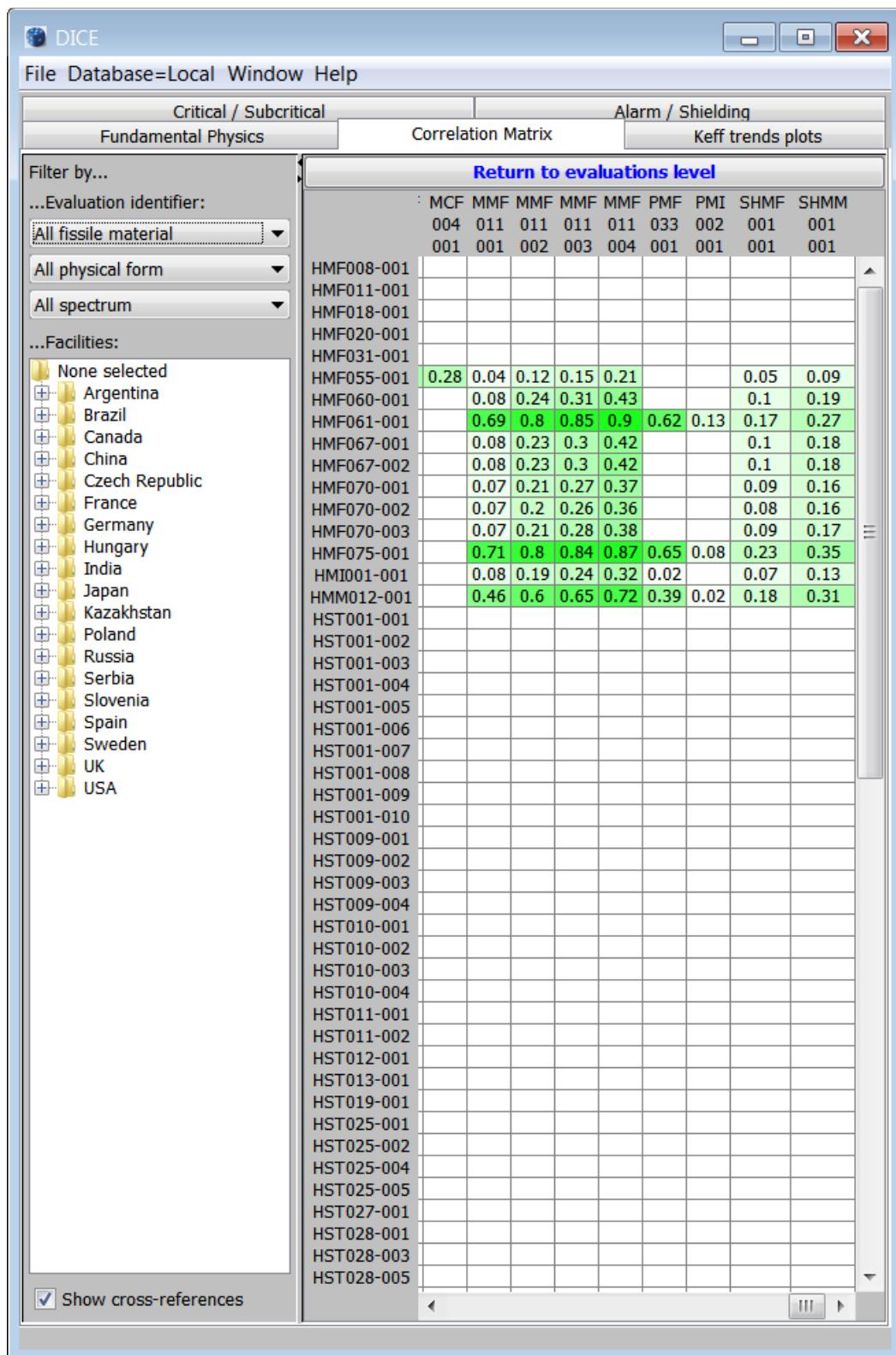
Critical / Subcritical	Alarm / Shielding	Fundamental Physics	Correlation Matrix	Keff trends plots
Return to evaluations level				
	HST 042 042 042 042 042 042 042 042 042 043 043 043 004 005			
	001 002 003 004 005 006 007 008 001 002 003 001 002 003 001 001			
Filter by...	HMF008-001			
...Evaluation identifier:	HMF011-001			
All fissile material	HMF018-001			
All physical form	HMF020-001			
All spectrum	HMF031-001			
...Facilities:	HMF055-001			
None selected	HMF060-001			
+ Argentina	HMF061-001			
+ Brazil	HMF067-001			
+ Canada	HMF067-002			
+ China	HMF070-001			
+ Czech Republic	HMF070-002			
+ France	HMF070-003			
+ Germany	HMF075-001			
+ Hungary	HMI001-001			
+ India	HMM012-001			
+ Japan	HST001-001			
+ Kazakhstan	HST001-002			
+ Poland	HST001-003			
+ Russia	HST001-004			
+ Serbia	HST001-005			
+ Slovenia	HST001-006			
+ Spain	HST001-007			
+ Sweden	HST001-008			
+ UK	HST001-009			
+ USA	HST001-010			
	HST009-001			
	HST009-002			
	HST009-003			
	HST009-004			
	HST010-001			
	HST010-002			
	HST010-003			
	HST010-004			
	HST011-001			
	HST011-002			
	HST012-001			
	HST013-001	0.29 0.31 0.38 0.36 0.37 0.35 0.36 0.35		0.11
	HST019-001			
	HST025-001			
	HST025-002			
	HST025-004			
	HST025-005			
	HST027-001			
	HST028-001			
	HST028-003			
	HST028-005			
<input checked="" type="checkbox"/> Show cross-references				

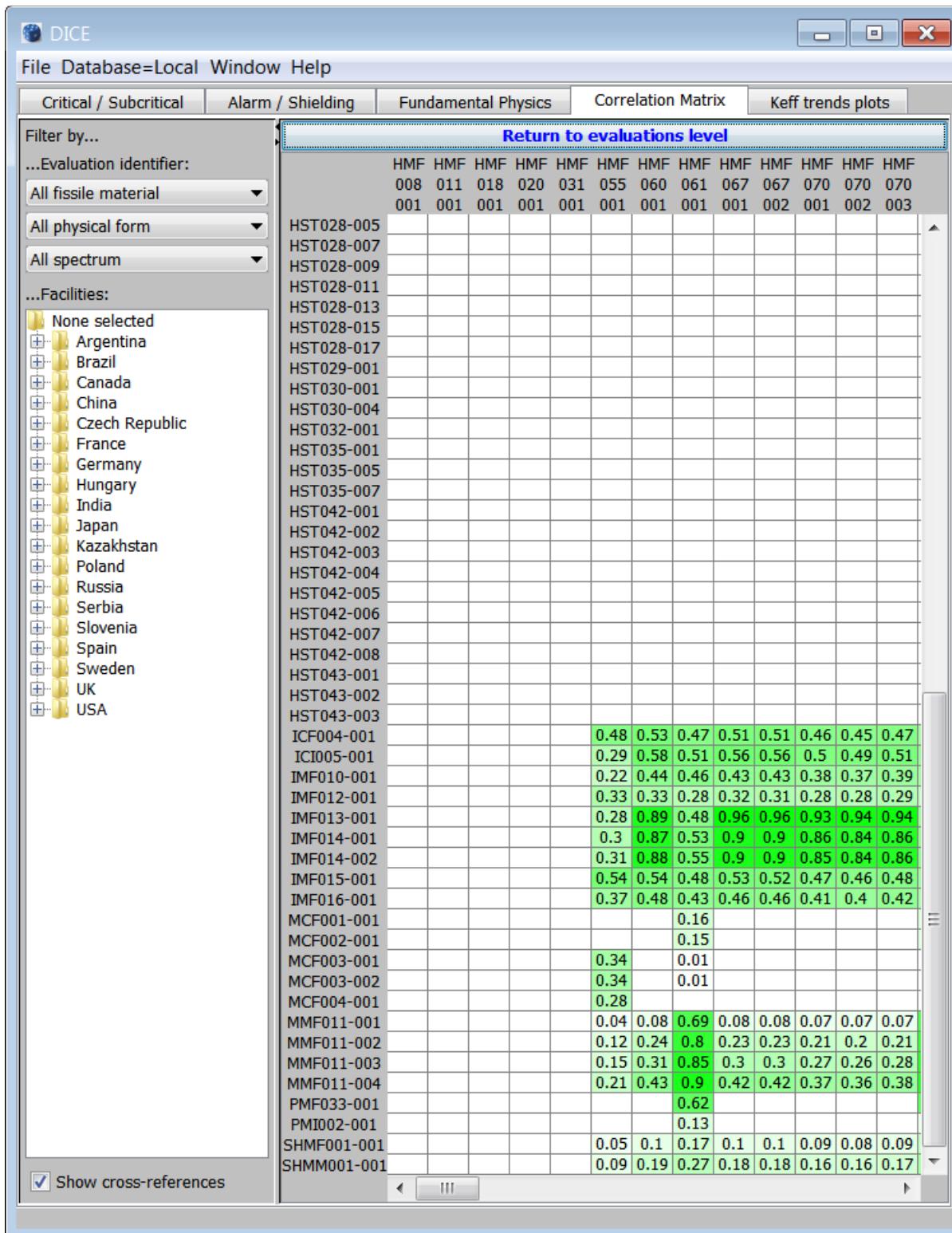
DICE

File Database=Local Window Help

	ICI	IMF	IMF	IMF	IMF	IMF	IMF	MCF	MCF	MCF	MCF	MCF
005	010	012	013	014	014	015	016	001	002	003	003	004
001	001	001	001	001	002	001	001	001	001	001	002	001
HMF008-001												
HMF011-001												
HMF018-001												
HMF020-001												
HMF031-001												
HMF055-001	0.29	0.22	0.33	0.28	0.3	0.31	0.54	0.37			0.34	0.34
HMF060-001	0.58	0.44	0.33	0.89	0.87	0.88	0.54	0.48				
HMF061-001	0.51	0.46	0.28	0.48	0.53	0.55	0.48	0.43	0.16	0.15	0.01	0.01
HMF067-001	0.56	0.43	0.32	0.96	0.9	0.9	0.53	0.46				
HMF067-002	0.56	0.43	0.31	0.96	0.9	0.9	0.52	0.46				
HMF070-001	0.5	0.38	0.28	0.93	0.86	0.85	0.47	0.41				
HMF070-002	0.49	0.37	0.28	0.94	0.84	0.84	0.46	0.4				
HMF070-003	0.51	0.39	0.29	0.94	0.86	0.86	0.48	0.42				
HMF075-001	0.42	0.36	0.23	0.4	0.43	0.45	0.38	0.34	0.13	0.12		
HMI001-001	0.41	0.31	0.23	0.76	0.67	0.67	0.38	0.33				
HMM012-001	0.52	0.4	0.29	0.5	0.55	0.57	0.48	0.42	0.03	0.03		
HST001-001												
HST001-002												
HST001-003												
HST001-004												
HST001-005												
HST001-006												
HST001-007												
HST001-008												
HST001-009												
HST001-010												
HST009-001												
HST009-002												
HST009-003												
HST009-004												
HST010-001												
HST010-002												
HST010-003												
HST010-004												
HST011-001												
HST011-002												
HST012-001												
HST013-001												
HST019-001												
HST025-001												
HST025-002												
HST025-004												
HST025-005												
HST027-001												
HST028-001												
HST028-003												
HST028-005												

Show cross-references





DICE

File Database=Local Window Help

Critical / Subcritical	Alarm / Shielding	Fundamental Physics	Correlation Matrix	Keff trends plots									
Filter by... ...Evaluation identifier: All fissile material All physical form All spectrum ...Facilities:  None selected Argentina Brazil Canada China Czech Republic France Germany Hungary India Japan Kazakhstan Poland Russia Serbia Slovenia Spain Sweden UK USA													
Return to evaluations level													
HMF	HMF	HMI	HMM	HST	HST	HST	HST	HST	HST	HST	HST	HST	HST
070	075	001	012	001	001	001	001	001	001	001	001	001	001
003	001	001	001	001	002	003	004	005	006	007	008	009	
HST028-005													
HST028-007													
HST028-009													
HST028-011													
HST028-013													
HST028-015													
HST028-017													
HST029-001													
HST030-001													
HST030-004													
HST032-001													
HST035-001													
HST035-005													
HST035-007													
HST042-001													
HST042-002													
HST042-003													
HST042-004													
HST042-005													
HST042-006													
HST042-007													
HST042-008													
HST043-001													
HST043-002													
HST043-003													
ICF004-001	0.47	0.37	0.37	0.47									
ICI005-001	0.51	0.42	0.41	0.52									
IMF010-001	0.39	0.36	0.31	0.4									
IMF012-001	0.29	0.23	0.23	0.29									
IMF013-001	0.94	0.4	0.76	0.5									
IMF014-001	0.86	0.43	0.67	0.55									
IMF014-002	0.86	0.45	0.67	0.57									
IMF015-001	0.48	0.38	0.38	0.48									
IMF016-001	0.42	0.34	0.33	0.42									
MCF001-001		0.13		0.03									
MCF002-001		0.12		0.03									
MCF003-001													
MCF003-002													
MCF004-001													
MMF011-001	0.07	0.71	0.08	0.46									
MMF011-002	0.21	0.8	0.19	0.6									
MMF011-003	0.28	0.84	0.24	0.65									
MMF011-004	0.38	0.87	0.32	0.72									
PMF033-001		0.65	0.02	0.39									
PMI002-001		0.08		0.02									
SHMF001-001	0.09	0.23	0.07	0.18									
SHMM001-001	0.17	0.35	0.13	0.31									

Show cross-references

The screenshot shows the DICE software interface with a correlation matrix table. The table has 15 columns and 30 rows, labeled HST 001 through HST 012, and ICF004-001 through SHMM001-001. The first three rows of the table contain numerical values: 0.13, 0.14, 0.12; 0.1, 0.08, 0.08; and 0.08, 0.47, 0.47 respectively. The remaining rows are mostly empty or contain placeholder text like 'None selected' or facility names.

	HST 001	HST 002	HST 003	HST 004	HST 005	HST 006	HST 007	HST 008	HST 009	HST 010	HST 011	HST 012	
HST028-005	0.13	0.14	0.12	0.1	0.08	0.08	0.08	0.08	0.47	0.47	0.05		
HST028-007	0.29	0.25	0.19	0.13	0.12	0.12	0.12	0.12	0.12	0.24	0.24	0.47	
HST028-009	0.29	0.26	0.19	0.13	0.12	0.12	0.12	0.12	0.12	0.25	0.25	0.36	
HST028-011													
HST028-013													
HST028-015													
HST028-017													
HST029-001													
HST030-001													
HST030-004													
HST032-001													
HST035-001													
HST035-005													
HST035-007													
HST042-001													
HST042-002													
HST042-003													
HST042-004													
HST042-005													
HST042-006													
HST042-007													
HST042-008													
HST043-001													
HST043-002													
HST043-003													
ICF004-001													
ICIO05-001													
IMF010-001													
IMF012-001													
IMF013-001													
IMF014-001													
IMF014-002													
IMF015-001													
IMF016-001													
MCF001-001													
MCF002-001													
MCF003-001													
MCF003-002													
MCF004-001													
MMF011-001													
MMF011-002													
MMF011-003													
MMF011-004													
PMF033-001													
PMI002-001													
SHMF001-001													
SHMM001-001													

DICE

File Database=Local Window Help

	Critical / Subcritical	Alarm / Shielding	Fundamental Physics	Correlation Matrix	Keff trends plots									
Filter by...	Return to evaluations level													
...Evaluation identifier:	HST 012 001	HST 013 001	HST 019 001	HST 025 002	HST 025 004	HST 025 005	HST 027 001	HST 028 001	HST 028 003	HST 028 005	HST 028 007	HST 028 009	HST 028 009	
All fissile material	0.2	0.16	0.16	0.14	0.12	0.3	0.43	0.41	1	0.32	0.47			
All physical form	0.16	0.12	0.12	0.11	0.09	0.81	0.31	0.29	0.32	1	0.33			
All spectrum	0.36	0.26	0.26	0.23	0.19	0.33	0.46	0.43	0.47	0.33	1			
...Facilities:	0.35	0.24	0.24	0.23	0.18	0.34	0.47	0.45	0.49	0.35	0.63			
None selected	0.33	0.24	0.24	0.21	0.18	0.33	0.65	0.43	0.48	0.34	0.61			
Argentina	0.31	0.22	0.22	0.2	0.17	0.3	0.42	0.39	0.74	0.3	0.56			
Brazil	0.32	0.22	0.22	0.2	0.17	0.77	0.36	0.34	0.36	0.81	0.5			
Canada	0.32	0.22	0.22	0.2	0.16	0.76	0.37	0.34	0.37	0.81	0.51			
China	0.15	0.12	0.12	0.1	0.09	0.82	0.28	0.26	0.28	0.87	0.3			
Czech Republic	0.29	0.21	0.21	0.19	0.16	0.78	0.37	0.34	0.37	0.83	0.47			
France	0.41													
Germany		0.34	0.32	0.32	0.3	0.22	0.22	0.36	0.33	0.34	0.24	0.43		
Hungary		0.17	0.14	0.14	0.12	0.11	0.15	0.21	0.2	0.21	0.16	0.25		
India		0.18	0.12	0.12	0.11	0.1	0.2	0.27	0.25	0.28	0.2	0.31		
Japan		0.29												
Kazakhstan		0.31												
Poland		0.38												
Russia		0.36												
Serbia		0.37												
Slovenia		0.35												
Spain		0.36												
Sweden		0.35												
UK		0.05												
USA		0.47												
		0.36	0.11											
ICF004-001														
ICIO05-001														
IMF010-001														
IMF012-001														
IMF013-001														
IMF014-001														
IMF014-002														
IMF015-001														
IMF016-001														
MCF001-001														
MCF002-001														
MCF003-001														
MCF003-002														
MCF004-001														
MMF011-001														
MMF011-002														
MMF011-003														
MMF011-004														
PMF033-001														
PMI002-001														
SHMF001-001														
SHMM001-001														
<input checked="" type="checkbox"/> Show cross-references														

DICE

File Database=Local Window Help

	Critical / Subcritical	Alarm / Shielding	Fundamental Physics	Correlation Matrix	Keff trends plots
Filter by...					
...Evaluation identifier:					
All fissile material	028	028	028	028	028
	009	011	013	015	017
	HST028-005	0.47	0.49	0.48	0.74
	HST028-007	0.33	0.35	0.34	0.3
	HST028-009	1	0.63	0.61	0.56
	HST028-011	0.63	1	0.62	0.57
	HST028-013	0.61	0.62	1	0.56
	HST028-015	0.56	0.57	0.56	1
	HST028-017	0.5	0.5	0.49	0.45
	HST029-001	0.51	0.51	0.5	0.46
	HST030-001	0.3	0.31	0.29	0.27
	HST030-004	0.47	0.48	0.47	0.42
	HST032-001	0.47	0.48	0.47	0.42
	HST035-001	0.43	0.42	0.41	0.37
	HST035-005	0.25	0.25	0.24	0.22
	HST035-007	0.31	0.32	0.32	0.28
	HST042-001				
	HST042-002				
	HST042-003				
	HST042-004				
	HST042-005				
	HST042-006				
	HST042-007				
	HST042-008				
	HST043-001				
	HST043-002				
	HST043-003				
	ICF004-001				
	ICIO05-001				
	IMF010-001				
	IMF012-001				
	IMF013-001				
	IMF014-001				
	IMF014-002				
	IMF015-001				
	IMF016-001				
	MCF001-001				
	MCF002-001				
	MCF003-001				
	MCF003-002				
	MCF004-001				
	MMF011-001				
	MMF011-002				
	MMF011-003				
	MMF011-004				
	PMF033-001				
	PMI002-001				
	SHMF001-001				
	SHMM001-001				

Show cross-references

DICE

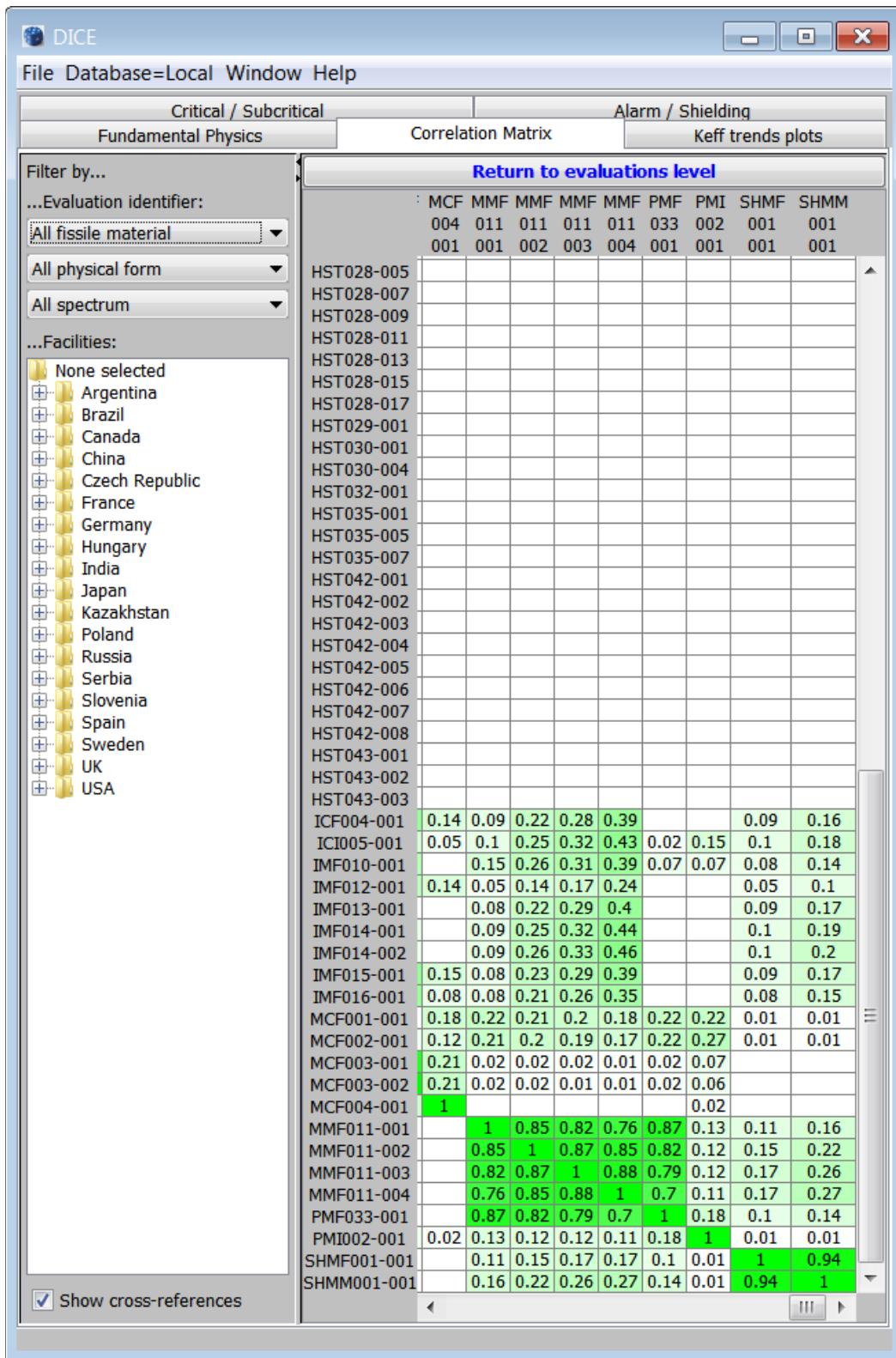
File Database=Local Window Help

Critical / Subcritical	Alarm / Shielding	Fundamental Physics	Correlation Matrix	Keff trends plots																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
Return to evaluations level <table border="1"> <thead> <tr> <th>HST</th> <th>ICF</th> <th>ICI</th> </tr> <tr> <th>042</th> <th>042</th> <th>042</th> <th>042</th> <th>042</th> <th>042</th> <th>042</th> <th>042</th> <th>043</th> <th>043</th> <th>043</th> <th>004</th> <th>005</th> </tr> <tr> <th>001</th> <th>002</th> <th>003</th> <th>004</th> <th>005</th> <th>006</th> <th>007</th> <th>008</th> <th>001</th> <th>002</th> <th>003</th> <th>001</th> <th>001</th> </tr> </thead> <tbody> <tr> <td>HST028-005</td> <td></td> </tr> <tr> <td>HST028-007</td> <td></td> </tr> <tr> <td>HST028-009</td> <td></td> </tr> <tr> <td>HST028-011</td> <td></td> </tr> <tr> <td>HST028-013</td> <td></td> </tr> <tr> <td>HST028-015</td> <td></td> </tr> <tr> <td>HST028-017</td> <td></td> </tr> <tr> <td>HST029-001</td> <td></td> </tr> <tr> <td>HST030-001</td> <td></td> </tr> <tr> <td>HST030-004</td> <td></td> </tr> <tr> <td>HST032-001</td> <td>0.31</td> <td>0.35</td> <td>0.42</td> <td>0.42</td> <td>0.42</td> <td>0.38</td> 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ICF004-001	0.65	0.82	0.52	0.51	0.69	0.67	0.91	0.91		0.4	0.41	0.14																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
ICI005-001	1	0.69	0.38	0.54	0.65	0.66	0.63	0.64	0.36	0.36	0.16	0.16	0.05																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
IMF010-001	0.69	1	0.44	0.44	0.65	0.62	0.75	0.91	0.1	0.1	0.28	0.28																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
IMF012-001	0.38	0.44	1	0.31	0.4	0.39	0.52	0.51			0.27	0.27	0.14																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
IMF013-001	0.54	0.44	0.31	1	0.97	0.93	0.52	0.47			0.01	0.01																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
IMF014-001	0.65	0.65	0.4	0.97	1	0.96	0.67	0.68			0.1	0.1																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
IMF014-002	0.66	0.62	0.39	0.93	0.96	1	0.66	0.65			0.07	0.07																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
IMF015-001	0.63	0.75	0.52	0.52	0.67	0.66	1	0.86			0.41	0.42	0.15																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
IMF016-001	0.64	0.91	0.51	0.47	0.68	0.65	0.86	1			0.39	0.4	0.08																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
MCF001-001	0.36	0.1							1	0.66			0.18																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
MCF002-001	0.36	0.1							0.66	1	0.07	0.06	0.12																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
MCF003-001	0.16	0.28	0.27	0.01	0.1	0.07	0.41	0.39		0.07	1	0.85	0.21																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
MCF003-002	0.16	0.28	0.27	0.01	0.1	0.07	0.42	0.4		0.06	0.85	1	0.21																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
MCF004-001	0.05		0.14				0.15	0.08	0.18	0.12	0.21	0.21	1																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
MMF011-001	0.1	0.15	0.05	0.08	0.09	0.09	0.08	0.08	0.22	0.21	0.02	0.02																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
MMF011-002	0.25	0.26	0.14	0.22	0.25	0.26	0.23	0.21	0.2	0.2	0.02	0.02																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
MMF011-003	0.32	0.31	0.17	0.29	0.32	0.33	0.29	0.26	0.2	0.19	0.02	0.01																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
MMF011-004	0.43	0.39	0.24	0.4	0.44	0.46	0.39	0.35	0.18	0.17	0.01	0.01																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
PMF033-001	0.02	0.07							0.22	0.22	0.02	0.02																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
PMI002-001	0.15	0.07							0.22	0.27	0.07	0.06	0.02																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
SHMF001-001	0.1	0.08	0.05	0.09	0.1	0.1	0.09	0.08	0.01	0.01																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
SHMM001-001	0.18	0.14	0.1	0.17	0.19	0.2	0.17	0.15	0.01	0.01																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										



APPENDIX G – Cross Reference for Isotopes in the
ORNL Covariance Data and MCNP6 Cross Section Library

The following table lists the ZA values in the ORNL covariance data which have a corresponding S(α,β) identifier in the MCNP6 cross section library.

SCALE ZA Identifier	Description ^(a)	MCNP6 S(α,β) Identifier	Description ^(b)
1001	Hydrogen in water with a S(α,β) thermal kernel	lwtr	Hydrogen in Light Water
1701	Hydrogen in zirconium hydride with a S(α,β) thermal kernel	h-zr	Hydrogen in Zirconium Hydride
1801	Hydrogen with a free gas thermal kernel	1001	elemental H-1
1901	Hydrogen in polyethylene with a S(α,β) thermal kernel	poly	Hydrogen in Polyethylene
1002	Deuterium in heavy water with S(α,β) thermal kernel	hwtr	Deuterium in Heavy Water
1802	Deuterium with a free gas thermal kernel	1002	elemental H-2
4309	Beryllium metal with a S(α,β) thermal kernel	be	Beryllium Metal
6312	Graphite carbon	grph	Graphite

^(a) ORNL/TM-2005/39; Table M8.2.3, Elements and special nuclide symbols, Table M8.2.4, Compounds, and Section M4.A.2, The 44-Group ENDF/B-V Library

^(b) LA-UR-13-21822; Table 7: Thermal S(α,β) cross-section libraries, and Table 8: continuous-energy neutron data library

Zirconium in Zirconium Hydride

ORNL/TM-2005/39, Section M4.A.2, lists zirconium in zirconium hydride with a ZA of 40701. The MCNP6 cross section library also has zirconium in zirconium hydride (with the identifiers is zr-h and zr/h). However, the native covariance file ORNL_SCAL6.1.cov does not have a material with the ZA 40701, which is why ZA 40701 is not in the table above (or script file ProcessCovData.csh).

Meta-Stable Isotopes (and Americium-242)

The ORNL covariance data and the MCNP6 library have different notations for meta-stable isotopes. The MCNP6 library provides both the ZA and SZAX identifiers for isotopes; the choice depends on the library being used. (The ZA suffixes are used with the 8xc libraries and the SZA extensions are used with the 71xnc libraries where x ranges from 0–6 and refers to the

temperatures to which the evaluations were processed.) The following table lists the ORNL ZA identifiers with the MCNP6 ZA and SZAX identifiers.

In addition, an exception to the ZA and SZA construction formulas occurs with Am-242. For many years, the first excited state for Am-242 (i.e., Am-242m) was the only available evaluation and 95242 was used to identify it. (The first excited state has a half-life of 141 yr while the ground state has a half-life of 16.02 h.) When the ground state evaluation was first made available, the ZA of 95642 was assigned to Am-242 to maintain backwards compatibility. For Am-242, 95242 refers to the first excited state evaluation and 95642 refers to the ground state evaluation - the reverse of the convention. [LA-UR-13-20137; Sec. 1.1]

	ORNL Covariance Data Isotope	SCALE ZA Identifier ^(c)	MCNP6 Library ZA Identifier ^(d)	MCNP6 Library SZAX Identifier ^(d)
1.	Co-58m	27601	27458	1027058
2.	Ag-110m	47601	47510	1047110
3.	Cd-115m	48601	48515	1048115
4.	Te-127m	52601	52527	1052127
5.	Te-129m	52611	52529	1052129
6.	Pm-148m	61601	61548	1061148
7.	Ho-166m	67601	67566	1067166
8.	Am-242	95242	95642	1095242
9.	Am-242m	95601	95242	95242
10.	Am-244m	95611	95644	1095244

^(c) ORNL/TM-2005/39; Table M8.2.1, Isotopes in standard composition library

^(d) LA-UR-13-20137; Table 2 (plus corrections to ZA identifiers according to ZA formula and LA-UR-13-21822)

All of the SCALE ZA identifiers are used in the ORNL covariance data library. Whisper V1.0.0 (script file ProcessCovData.csh) does not translate any of these files to the MCNP6 identifiers.

The benchmark models distributed with Whisper V1.0.0 were searched for the isotopes listed above. None of the benchmark models include any of the listed isotopes. Therefore, the fact that the covariance data for these isotopes is missing or incorrect does not affect the final results for any application model. The supporting information for this conclusion is:

1. The covariances and variances [LA-UR-14-26558; eq. 30 and 31] with the benchmarks sensitivity vectors are not effected because the benchmark sensitivity coefficients for these isotopes are zero.
2. The presence (or lack) of covariance data could change the variances [LA-UR-14-26558; eq. 31] of the applications (i.e., with the application sensitivity vectors) and the resulting

correlation coefficients [LA-UR-14-26558; eq. 32]. However, any influence on the correlation coefficients is cancelled when the weighting factors [LA-UR-14-26558; eq. 34] are calculated.

MCNP6 Library ZA Identifier

The ZAID looks like [LA-UR-13-20137; eq. 1]:

ZZZAAA.ddt

where

ZZZ the atomic number (blank padded, not zero padded if the atomic number < 100),
 AAA the atomic mass number,
 dd the library identifier,
 t table type.

For nuclides in an ACE table (e.g., MCNP6 library) , the ZA of isotopes in the ground states is [LA-UR-13-20137; eq. 2]:

$$ZA = 1000 \times Z + A$$

For nuclides in an ACE table (e.g., MCNP6 library) , the ZA of isotopes in an excited states is [LA-UR-13-20137; eq. 3]:

$$ZA = 1000 \times Z + 300 + s \times 100 + A$$

where s is the excited state of the evaluated isotopes; $s = 0$ for the ground state, $s = 1$ for the first excited state, etc.

A historical exception to the ZA construction formula is Am-242. For many years, the first excited state for Am-242 (i.e., Am-242m) was the only available evaluation and 95242 was used to identify it. (The first excited state has a half-life of 141 yr while the ground state has a half-life of 16.02 h.) When the ground state evaluation was first made available, the ZA of 95642 was assigned to Am-242 to maintain backwards compatibility. For Am-242, 95242 refers to the first excited state evaluation and 95642 refers to the ground state evaluation - the reverse of the convention. [LA-UR-13-20137; Sec. 1.1]

MCNP6 Library SZAX Identifier

For nuclides in an ACE table (e.g., MCNP6 library) , the SZA of isotopes is [LA-UR-13-20137; eq. 5]:

$$SZA = S \times 10^6 + Z \times 10^3 + A$$

References

LA-UR-13-20137, *Continuous Energy Neutron Cross Section Data Tables Based upon ENDF/B-VII.1*, February 14, 2013

LA-UR-13-21822, Version 1, *Listing of Available ACE Data Tables*, 2013-06-05

ORNL/TM-2005/39, Version 6.1, *SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, June 2011

APPENDIX H – File cov.lwtr.dat

The following is a condensed listing of the base covariance data file ‘cov.lwtr.dat’. Notice that the lines are not consecutive between the following pages.

```

1      lwtr      44      5
2      2.0000E+07  8.1873E+06  6.4340E+06  4.8000E+06  3.0000E+06
3      2.4790E+06  2.3540E+06  1.8500E+06  1.4000E+06  9.0000E+05  4.0000E+05
4      1.0000E+05  2.5000E+04   1.7000E+04   3.0000E+03  5.5000E+02  1.0000E+02
5      3.0000E+01   1.0000E+01   8.1000E+00   6.0000E+00  4.7500E+00  3.0000E+00
6      1.7700E+00   1.0000E+00   6.2500E-01   4.0000E-01  3.7500E-01  3.5000E-01
7      3.2500E-01   2.7500E-01   2.5000E-01   2.2500E-01  2.0000E-01  1.5000E-01
8      1.0000E-01   7.0000E-02   5.0000E-02   4.0000E-02  3.0000E-02  2.5300E-02
9      1.0000E-02   7.5000E-03   3.0000E-03   1.0000E-05
10     lwtr      1      lwtr      1
11     lwtr      1      lwtr      2
12     lwtr      1      lwtr      102
13     lwtr      2      lwtr      2
14     lwtr      102     lwtr      102
15     lwtr      1      lwtr      1      1
16     44       1       44       2       44       3       44       4       44       5       44       6
17     44       7       44       8       44       9       44       10      44       11      44       12
18     44       13      44       14      44       15      44       16      44       17      44       18
19     44       19      44       20      44       21      44       22      44       23      44       24
20     44       25      44       26      44       27      44       28      44       29      44       30
21     44       31      44       32      44       33      44       34      44       35      44       36
22     44       37      44       38      44       39      44       40      44       41      44       42
23     44       43      44       44
24      2.7701E-04  4.2241E-04  3.9348E-04  3.3522E-04  2.9687E-04  2.9687E-04
25      2.7387E-04  2.1960E-04  2.0729E-04  1.4204E-04  7.8130E-05  4.8972E-05
26      4.8972E-05  4.1975E-05  0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
27      0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
28      0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
29      0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
30      0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
31      0.0000E+00   0.0000E+00   4.2241E-04  6.4432E-04  6.0021E-04  5.1136E-04
...
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...

337	9.8357E-07	9.8342E-07	9.8326E-07	9.8293E-07	9.8232E-07	9.8165E-07							
338	9.8102E-07	9.8051E-07	9.8007E-07	9.7969E-07	9.7904E-07	9.7833E-07							
339	9.7801E-07	9.7762E-07	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
340	0.0000E+00												
341	0.0000E+00	0.0000E+00	0.0000E+00	2.4230E-07	1.5656E-06	9.8601E-07							
342	9.8590E-07	9.8572E-07	9.8557E-07	9.8550E-07	9.8541E-07	9.8528E-07							
343	9.8504E-07	9.8470E-07	9.8429E-07	9.8385E-07	9.8356E-07	9.8348E-07							
344	9.8339E-07	9.8324E-07	9.8306E-07	9.8292E-07	9.8276E-07	9.8244E-07							
345	9.8184E-07	9.8119E-07	9.8057E-07	9.8007E-07	9.7964E-07	9.7927E-07							
346	9.7863E-07	9.7794E-07	9.7762E-07	9.7725E-07									
347		lwtr	1	lwtr	2	1							
348		44	1	44	2	44	3	44	4	44	5	44	6
349		44	7	44	8	44	9	44	10	44	11	44	12
350		44	13	44	14	44	15	44	16	44	17	44	18
351		44	19	44	20	44	21	44	22	44	23	44	24
352		44	25	44	26	44	27	44	28	44	29	44	30
353		44	31	44	32	44	33	44	34	44	35	44	36
354		44	37	44	38	44	39	44	40	44	41	44	42
355		44	43	44	44								
356			2.7702E-04		4.2243E-04		3.9349E-04		3.3523E-04		2.9687E-04		2.9688E-04
357			2.7388E-04		2.1961E-04		2.0729E-04		1.4204E-04		7.8132E-05		4.8974E-05
358			4.8973E-05		4.1977E-05		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
359			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
360			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
361			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
362			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
363			0.0000E+00		0.0000E+00		4.2242E-04		6.4433E-04		6.0023E-04		5.1138E-04
364			4.5288E-04		4.5288E-04		4.1781E-04		3.3505E-04		3.1626E-04		2.1671E-04
365			1.1920E-04		7.4705E-05		7.4704E-05		6.4031E-05		0.0000E+00		0.0000E+00

...

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669	9.9521E-07	9.9499E-07	9.9473E-07	9.9423E-07	9.9331E-07	9.9228E-07								
670	9.9131E-07	9.9053E-07	9.8985E-07	9.8928E-07	9.8828E-07	9.8720E-07								
671	9.8670E-07	9.8612E-07	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00								
672	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00								
673	0.0000E+00	0.0000E+00	0.0000E+00	2.4571E-07	1.5876E-06	9.9983E-07								
674	9.9965E-07	9.9937E-07	9.9914E-07	9.9903E-07	9.9888E-07	9.9867E-07								
675	9.9830E-07	9.9778E-07	9.9714E-07	9.9644E-07	9.9599E-07	9.9587E-07								
676	9.9573E-07	9.9548E-07	9.9521E-07	9.9499E-07	9.9473E-07	9.9423E-07								
677	9.9331E-07	9.9228E-07	9.9131E-07	9.9053E-07	9.8985E-07	9.8928E-07								
678	9.8828E-07	9.8720E-07	9.8670E-07	9.8612E-07										
679		lwtr	1	lwtr	102	1								
680		44	1	44	2	44	3	44	4	44	5	44	6	
681		44	7	44	8	44	9	44	10	44	11	44	12	
682		44	13	44	14	44	15	44	16	44	17	44	18	
683		44	19	44	20	44	21	44	22	44	23	44	24	
684		44	25	44	26	44	27	44	28	44	29	44	30	
685		44	31	44	32	44	33	44	34	44	35	44	36	
686		44	37	44	38	44	39	44	40	44	41	44	42	
687		44	43	44	44									
688			1.0256E-06	1.4573E-06	1.4904E-06	1.4272E-06	1.3131E-06	1.2219E-06						
689			1.1111E-06	9.3237E-07	6.9523E-07	3.2351E-07	5.9937E-08	-2.7841E-09						
690			-4.2342E-09	-6.2839E-09	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
691			0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
692			0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
693			0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
694			0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
695			0.0000E+00	0.0000E+00	1.7635E-06	2.5410E-06	2.6035E-06	2.4972E-06						
696			2.2995E-06	2.1397E-06	1.9479E-06	1.6390E-06	1.2237E-06	5.7512E-07						
697			1.1396E-07	5.7790E-09	8.7890E-09	1.3044E-08	0.0000E+00	0.0000E+00						

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1001	1.1982E-07	1.2534E-07	1.3171E-07	1.4418E-07	1.6738E-07	1.9309E-07							
1002	2.1728E-07	2.3680E-07	2.5364E-07	2.6802E-07	2.9298E-07	3.1991E-07							
1003	3.3238E-07	3.4692E-07	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00							
1004	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00							
1005	0.0000E+00	0.0000E+00	0.0000E+00	1.2133E-10	1.9424E-09	4.3228E-09							
1006	8.7896E-09	1.5697E-08	2.1480E-08	2.4266E-08	2.7896E-08	3.3161E-08							
1007	4.2398E-08	5.5533E-08	7.1556E-08	8.8994E-08	1.0013E-07	1.0329E-07							
1008	1.0680E-07	1.1288E-07	1.1982E-07	1.2534E-07	1.3171E-07	1.4418E-07							
1009	1.6738E-07	1.9309E-07	2.1728E-07	2.3680E-07	2.5364E-07	2.6802E-07							
1010	2.9298E-07	3.1991E-07	3.3238E-07	3.4692E-07									
1011		lwtr	2	lwtr	2	1							
1012		44	1	44	2	44	3	44	4	44	5	44	6
1013		44	7	44	8	44	9	44	10	44	11	44	12
1014		44	13	44	14	44	15	44	16	44	17	44	18
1015		44	19	44	20	44	21	44	22	44	23	44	24
1016		44	25	44	26	44	27	44	28	44	29	44	30
1017		44	31	44	32	44	33	44	34	44	35	44	36
1018		44	37	44	38	44	39	44	40	44	41	44	42
1019		44	43	44	44								
1020			2.7703E-04		4.2244E-04		3.9350E-04		3.3523E-04		2.9688E-04		2.9688E-04
1021			2.7388E-04		2.1961E-04		2.0730E-04		1.4204E-04		7.8133E-05		4.8974E-05
1022			4.8974E-05		4.1978E-05		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1023			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1024			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1025			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1026			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1027			0.0000E+00		0.0000E+00		4.2244E-04		6.4435E-04		6.0024E-04		5.1138E-04
1028			4.5289E-04		4.5289E-04		4.1782E-04		3.3505E-04		3.1626E-04		2.1671E-04
1029			1.1920E-04		7.4706E-05		7.4706E-05		6.4033E-05		0.0000E+00		0.0000E+00

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1333	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06						
1334	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06						
1335	1.0000E-06	1.0000E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
1336	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
1337	0.0000E+00	0.0000E+00	0.0000E+00	2.4571E-07	1.5878E-06	1.0000E-06							
1338	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
1339	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
1340	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
1341	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
1342	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
1343		lwtr	102	lwtr	102	1							
1344		44	1	44	2	44	3	44	4	44	5	44	6
1345		44	7	44	8	44	9	44	10	44	11	44	12
1346		44	13	44	14	44	15	44	16	44	17	44	18
1347		44	19	44	20	44	21	44	22	44	23	44	24
1348		44	25	44	26	44	27	44	28	44	29	44	30
1349		44	31	44	32	44	33	44	34	44	35	44	36
1350		44	37	44	38	44	39	44	40	44	41	44	42
1351		44	43	44	44								
1352			3.1564E-02		5.4271E-02		6.5334E-02		7.8197E-02		8.5594E-02		8.5594E-02
1353			8.5578E-02		8.5539E-02		8.0857E-02		5.1569E-02		9.3256E-03		-2.3306E-04
1354			-2.3306E-04		-1.9977E-04		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1355			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1356			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1357			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1358			0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00		0.0000E+00
1359			0.0000E+00		0.0000E+00		5.4271E-02		9.4629E-02		1.1413E-01		1.3683E-01
1360			1.4989E-01		1.4989E-01		1.5003E-01		1.5036E-01		1.4232E-01		9.1678E-02
1361			1.7732E-02		4.8377E-04		4.8377E-04		4.1466E-04		0.0000E+00		0.0000E+00

...
1665 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05
1666 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05
1667 2.5000E-05 2.5000E-05 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
1668 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
1669 0.0000E+00 0.0000E+00 0.0000E+00 3.8570E-06 2.6218E-05 2.5000E-05
1670 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05
1671 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05
1672 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05
1673 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05
1674 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05 2.5000E-05

[End of file]

APPENDIX I – File ORNL_SCALE6.1.cov

The following is a condensed listing of the native covariance data file ‘ORNL_SCALE6.1.cov’. All blocks of data related to material 1001 (hydrogen) are listed below. Notice that the lines are not consecutive between the following pages.

```

1   0v v7rec ornl-10/2008      1
2   1d    44    44    0     2   2589   2558      3
3   2d coverx file for v7
4   3d  2.0000E+07  8.1873E+06  6.4340E+06  4.8000E+06  3.0000E+06
5   2.4790E+06  2.3540E+06  1.8500E+06  1.4000E+06  9.0000E+05  4.0000E+05
6   1.0000E+05  2.5000E+04  1.7000E+04  3.0000E+03  5.5000E+02  1.0000E+02
7   3.0000E+01  1.0000E+01  8.1000E+00  6.0000E+00  4.7500E+00  3.0000E+00
8   1.7700E+00  1.0000E+00  6.2500E-01  4.0000E-01  3.7500E-01  3.5000E-01
9   3.2500E-01  2.7500E-01  2.5000E-01  2.2500E-01  2.0000E-01  1.5000E-01
10  1.0000E-01  7.0000E-02  5.0000E-02  4.0000E-02  3.0000E-02  2.5300E-02
11  1.0000E-02  7.5000E-03  3.0000E-03  1.0000E-05
12  5d    1801    2     4    1801    102     4    1801     1     4    1802     1     4
13  1802    2     4    1802    102     4    1802    16     4    1003     1     4
14  1003    16     4    1003     2     4    2003     1     4    2003     2     4
...
646  1001    2     4    1001    102     4    1001     1     4    1701     2     4
...

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863187	7d	1001	2	1001	2	1							
863188	8d	44	1	44	2	44	3	44	4	44	5	44	6
		44	7	44	8	44	9	44	10	44	11	44	12
		44	13	44	14	44	15	44	16	44	17	44	18
		44	19	44	20	44	21	44	22	44	23	44	24
		44	25	44	26	44	27	44	28	44	29	44	30
		44	31	44	32	44	33	44	34	44	35	44	36
		44	37	44	38	44	39	44	40	44	41	44	42
863195		44	43	44	44								
863196	9d	2.7703E-04	4.2244E-04	3.9350E-04	3.3523E-04	2.9688E-04	2.9688E-04						
		2.7388E-04	2.1961E-04	2.0730E-04	1.4204E-04	7.8133E-05	4.8974E-05						
		4.8974E-05	4.1978E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
		0.0000E+00	0.0000E+00	4.2244E-04	6.4435E-04	6.0024E-04	5.1138E-04						
		4.5289E-04	4.5289E-04	4.1782E-04	3.3505E-04	3.1626E-04	2.1671E-04						
863205		1.1920E-04	7.4706E-05	7.4706E-05	6.4033E-05	0.0000E+00	0.0000E+00						

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863509	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06						
	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06						
	1.0000E-06	1.0000E-06	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00						
	0.0000E+00	0.0000E+00	0.0000E+00	2.4571E-07	1.5878E-06	1.0000E-06							
	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06							
863518	1.0000E-06	1.0000E-06	1.0000E-06	1.0000E-06									
863519	7d	1001	102	1001	102	1							
863520	8d	44	1	44	2	44	3	44	4	44	5	44	6
		44	7	44	8	44	9	44	10	44	11	44	12
		44	13	44	14	44	15	44	16	44	17	44	18
		44	19	44	20	44	21	44	22	44	23	44	24
		44	25	44	26	44	27	44	28	44	29	44	30
		44	31	44	32	44	33	44	34	44	35	44	36
		44	37	44	38	44	39	44	40	44	41	44	42
863527		44	43	44	44								
863528	9d	3.1564E-02	5.4271E-02	6.5334E-02	7.8197E-02	8.5594E-02	8.5594E-02						
		8.5578E-02	8.5539E-02	8.0857E-02	5.1569E-02	9.3256E-03	-2.3306E-04						
		-2.3306E-04	-1.9977E-04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00					
		0.0000E+00	0.0000E+00	5.4271E-02	9.4629E-02	1.1413E-01	1.3683E-01						
		1.4989E-01	1.4989E-01	1.5003E-01	1.5036E-01	1.4232E-01	9.1678E-02						
863537		1.7732E-02	4.8377E-04	4.8377E-04	4.1466E-04	0.0000E+00	0.0000E+00						

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864173	9.8357E-07	9.8342E-07	9.8326E-07	9.8293E-07	9.8232E-07	9.8165E-07	
	9.8102E-07	9.8051E-07	9.8007E-07	9.7969E-07	9.7904E-07	9.7833E-07	
	9.7801E-07	9.7762E-07	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
	0.0000E+00	0.0000E+00	0.0000E+00	2.4230E-07	1.5656E-06	9.8601E-07	
	9.8590E-07	9.8572E-07	9.8557E-07	9.8550E-07	9.8541E-07	9.8528E-07	
	9.8504E-07	9.8470E-07	9.8429E-07	9.8385E-07	9.8356E-07	9.8348E-07	
	9.8339E-07	9.8324E-07	9.8306E-07	9.8292E-07	9.8276E-07	9.8244E-07	
	9.8184E-07	9.8119E-07	9.8057E-07	9.8007E-07	9.7964E-07	9.7927E-07	
864182	9.7863E-07	9.7794E-07	9.7762E-07	9.7725E-07			
864183	7d	1001	1	1001	2	1	
864184	8d	44	1	44	2	44	3
		44	7	44	8	44	9
		44	13	44	14	44	15
		44	19	44	20	44	21
		44	25	44	26	44	27
		44	31	44	32	44	33
		44	37	44	38	44	39
		44	43	44	44	44	44
864191							
864192	9d	2.7702E-04	4.2243E-04	3.9349E-04	3.3523E-04	2.9687E-04	2.9688E-04
		2.7388E-04	2.1961E-04	2.0729E-04	1.4204E-04	7.8132E-05	4.8974E-05
		4.8973E-05	4.1977E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	4.2242E-04	6.4433E-04	6.0023E-04	5.1138E-04
		4.5288E-04	4.5288E-04	4.1781E-04	3.3505E-04	3.1626E-04	2.1671E-04
864201		1.1920E-04	7.4705E-05	7.4704E-05	6.4031E-05	0.0000E+00	0.0000E+00
...							

...							
864505	9.9521E-07	9.9499E-07	9.9473E-07	9.9423E-07	9.9331E-07	9.9228E-07	
	9.9131E-07	9.9053E-07	9.8985E-07	9.8928E-07	9.8828E-07	9.8720E-07	
	9.8670E-07	9.8612E-07	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
	0.0000E+00	0.0000E+00	0.0000E+00	2.4571E-07	1.5876E-06	9.9983E-07	
	9.9965E-07	9.9937E-07	9.9914E-07	9.9903E-07	9.9888E-07	9.9867E-07	
	9.9830E-07	9.9778E-07	9.9714E-07	9.9644E-07	9.9599E-07	9.9587E-07	
	9.9573E-07	9.9548E-07	9.9521E-07	9.9499E-07	9.9473E-07	9.9423E-07	
	9.9331E-07	9.9228E-07	9.9131E-07	9.9053E-07	9.8985E-07	9.8928E-07	
864514	9.8828E-07	9.8720E-07	9.8670E-07	9.8612E-07			
864515	7d	1001	1	1001	102	1	
864516	8d	44	1	44	2	44	3
		44	7	44	8	44	9
		44	13	44	14	44	15
		44	19	44	20	44	21
		44	25	44	26	44	27
		44	31	44	32	44	33
		44	37	44	38	44	39
		44	43	44	44	44	44
864523							
864524	9d	1.0256E-06	1.4573E-06	1.4904E-06	1.4272E-06	1.3131E-06	1.2219E-06
		1.1111E-06	9.3237E-07	6.9523E-07	3.2351E-07	5.9937E-08	-2.7841E-09
		-4.2342E-09	-6.2839E-09	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
		0.0000E+00	0.0000E+00	1.7635E-06	2.5410E-06	2.6035E-06	2.4972E-06
		2.2995E-06	2.1397E-06	1.9479E-06	1.6390E-06	1.2237E-06	5.7512E-07
864533		1.1396E-07	5.7790E-09	8.7890E-09	1.3044E-08	0.0000E+00	0.0000E+00
...							

...
864837 1.1982E-07 1.2534E-07 1.3171E-07 1.4418E-07 1.6738E-07 1.9309E-07
 2.1728E-07 2.3680E-07 2.5364E-07 2.6802E-07 2.9298E-07 3.1991E-07
 3.3238E-07 3.4692E-07 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
 0.0000E+00 0.0000E+00 0.0000E+00 1.2133E-10 1.9424E-09 4.3228E-09
 8.7896E-09 1.5697E-08 2.1480E-08 2.4266E-08 2.7896E-08 3.3161E-08
 4.2398E-08 5.5533E-08 7.1556E-08 8.8994E-08 1.0013E-07 1.0329E-07
 1.0680E-07 1.1288E-07 1.1982E-07 1.2534E-07 1.3171E-07 1.4418E-07
 1.6738E-07 1.9309E-07 2.1728E-07 2.3680E-07 2.5364E-07 2.6802E-07
864846 2.9298E-07 3.1991E-07 3.3238E-07 3.4692E-07

...
[End of File]

APPENDIX J – Comparison of cov.lwtr.dat and ORNL_SCALE6.1.cov

The following table compares files cov.lwtr.dat and ORNL_SCALE6.1.cov (Appendices T and U). Remember script file ProcessCovData.csh renames the file originally created as ‘cov.1001.dat’ to ‘cov.lwtr.cov’. Script file ProcessCovData.csh also changes the material identification from “1001” to “lwtr”. Other than the intentional change in material identification, no discrepancies between the two files were identified.

Line numbers in cov.lwtr.dat	Line numbers in ORNL_SCALE6.1.cov	Comparison
1	2	<p>The first line in the base covariance data file contains:</p> <ol style="list-style-type: none"> 1. Identification number for material 1 in the covariance data, which is also in the filename. For cov.lwtr.dat, this is “lwtr”. 2. Number of neutron energy groups, which is the 2nd value in the ‘1d’ line in ORNL_SCALE6.1.cov. 3. Number of blocks of covariance data for material 1, i.e., the number of ‘7d’ lines where material 1 is the first material. For cov.lwtr.dat, this is the number of ‘7d’ lines with “1001” as the first material.
2 – 9	4 – 11	<p>These cov.lwtr.dat lines list the neutron energy boundaries. Values are identical to the ORNL_SCALE6.1.cov data.</p> <p>(In COVERX files, ‘3d’ is the prefix for the neutron energy boundaries, see Table M18.A.8 in ORNL/TM-2005/39.)</p>
10	863851	<p>These cov.lwtr.dat lines list the identification numbers for material 1, reaction 1, material 2, and reaction 2. Other than the intentional change in material identification, the values are identical to the ORNL_SCALE6.1.cov data.</p> <p>(See Table M18.A.8 in ORNL/TM-2005/39 for the matrix control description.)</p>
11	864183	
12	864515	
13	863187	
14	863519	

Line numbers in cov.lwtr.dat	Line numbers in ORNL_SCALE6.1.cov	Comparison
15	863851	<p>This cov.lwtr.dat line begins the covariance data block for light water, reaction 1 with light water, reaction 1. The last value (1) is the number of data blocks. Other than the intentional change in material identification, the values are identical to the ORNL_SCALE6.1.cov data.</p> <p>(See Table M18.A.8 in ORNL/TM-2005/39 for the matrix control description.)</p>
16 – 23	863852 – 863859	<p>These lines are the block control data; see Table M18.A.8 in ORNL/TM-2005/39. The lines are identical except for the COVERX prefix ‘8d’.</p>
24 – 346	863860 – 864182	<p>These lines are the covariance matrix. The lines are identical except for the COVERX prefix ‘9d’.</p>
347	864183	<p>This cov.lwtr.dat line begins the covariance data block for light water, reaction 1 with light water, reaction 2. The last value (1) is the number of data blocks. Other than the intentional change in material identification, the values are identical to the ORNL_SCALE6.1.cov data.</p> <p>(See Table M18.A.8 in ORNL/TM-2005/39 for the matrix control description.)</p>
348 – 355	864184 – 864191	<p>These lines are the block control data; see Table M18.A.8 in ORNL/TM-2005/39. The lines are identical except for the COVERX prefix ‘8d’.</p>
356 – 678	864192 – 864514	<p>These lines are the covariance matrix. The lines are identical except for the COVERX prefix ‘9d’.</p>
679	864515	<p>This cov.lwtr.dat line begins the covariance data block for light water, reaction 1 with light water, reaction 102. The last value (1) is the number of data blocks. Other than the intentional change in material identification, the values are identical to the ORNL_SCALE6.1.cov data.</p> <p>(See Table M18.A.8 in ORNL/TM-2005/39 for the matrix control description.)</p>

Line numbers in cov.lwtr.dat	Line numbers in ORNL_SCALE6.1.cov	Comparison
680 – 687	864516 – 864523	These lines are the block control data; see Table M18.A.8 in ORNL/TM-2005/39. The lines are identical except for the COVERX prefix ‘8d’.
688 – 1010	864524 – 864846	These lines are the covariance matrix. The lines are identical except for the COVERX prefix ‘9d’.
1011	863187	This cov.lwtr.dat line begins the covariance data block for light water, reaction 2 with light water, reaction 2. The last value (1) is the number of data blocks. Other than the intentional change in material identification, the values are identical to the ORNL_SCALE6.1.cov data. (See Table M18.A.8 in ORNL/TM-2005/39 for the matrix control description.)
1012 – 1019	863188 – 863195	These lines are the block control data; see Table M18.A.8 in ORNL/TM-2005/39. The lines are identical except for the COVERX prefix ‘8d’.
1020 – 1342	863196 – 863518	These lines are the covariance matrix. The lines are identical except for the COVERX prefix ‘9d’.
1343	863519	This cov.lwtr.dat line begins the covariance data block for light water, reaction 102 with light water, reaction 102. The last value (1) is the number of data blocks. Other than the intentional change in material identification, the values are identical to the ORNL_SCALE6.1.cov data. (See Table M18.A.8 in ORNL/TM-2005/39 for the matrix control description.)
1344 – 1351	863520 – 86527	These lines are the block control data; see Table M18.A.8 in ORNL/TM-2005/39. The lines are identical except for the COVERX prefix ‘8d’.
1352 – 1674	863528 – 863850	These lines are the covariance matrix. The lines are identical except for the COVERX prefix ‘9d’.