SAND2021-9472

SANDIA REPORT
SAND20XX-XXXX
Printed November 2021

Sandia National Laboratories

MANIPULATE-2020: An Interface Tool for Nuclear Data Processing

Patrick J. Griffin

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico
87185 and Livermore,
California 94550

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology & Engineering Solutions of Sandia, LLC.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@osti.gov
Online ordering: http://www.osti.gov/scitech

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.gov
Online order: https://classic.ntis.gov/help/order-methods/

ABSTRACT

This report provides basic background data on the Manipulate-2020 code. This code is used for processing and "manipulation" of nuclear data in support of radiation metrology applications. The code is made available on the open GitHub repository and is available to the general nuclear data community.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

This page left blank

ACRONYMS AND DEFINITIONS

Abbreviation	Definition
DOE	Department of energy
ENDF	Evaluated Nuclear Data File
ESTSC	Energy Science and Technology Software Center
NEA	Nuclear Energy Agency
NTESS	Nuclear Technology and Engineering Solutions of Sandia
SNL	Sandia National Laboratories
WSL	Windows Subsystem for Linux

1. PURPOSE

The purpose of this document is to provide the basic information on then Manipulate-2020 code that is required to make it available to the general user community.

2. CODE RELEASE DOCUMENTATION

This section addresses the various aspects of the code and its release that are required for release by Sandia, with authorization from NTESS, through Energy Science and Technology Software Center (ESTSC), DOE's central software repository.

2.1. Software Name

MANIPULATE-2020

2.2. Software Version

Version 21-1

2.3. Author(s)

Patrick J. Griffin

2.4. Software Completion Date

June 15, 2021

2.5. Brief Description

Manipulate-2020 is a nuclear data manipulation code that interfaces with files output by the SNL-NJOY-2016 code and supports radiation metrology applications and material damage studies. Example applications include: a) the generation of tabular multigroup damage response functions from the SNL-NJOY-2016/GROUPR module; b) the weighting and combination of the NJOY-produced isotopic response functions to make elemental and material-specific damage response functions; c) the generation of uncertainty in spectrum-averaged metrics using either the spectrum or response covariance matrix; d) generation of correlation matrix data compatible with 2D plots using commercial software packages such as SigmaPlot; and e) testing and correction of correlation matrices to ensure that they are positive semidefinite and that spectrum correlation matrices obey the unity normalization constraint.

All of the modifications provided here are being made available to the GitHub-based repository for the Manipulate-2020 code. As additional useful enhancements are incorporated into the baseline Manipulate-2020 code, the radiation effects community will be able to use this expanded functionality in this nuclear data manipulation.

2.6. Practical Application

The software is used to "manipulate/process" nuclear data extracted from the Evaluated Nuclear Data Files (ENDF) used by the nuclear data community. This processing supports the development of energy-dependent damage response functions and other metrics that can be used to support the characterization radiation damage to materials, e.g., metal embrittlement of reactor pressure vessels.

2.7. Method of Solution

This software interfaces the information found in publicly available nuclear data evaluations, i.e., ENDF/B-VIII-0, with basic physics-related models supported by NJOY code processing for material damage, e.g., arc-dpa formulation found in NEA/NSC/DOC(2015)9. So, the "method of solution" is simple data manipulation according to defined physics relationships.

2.8. Computer(s) and Operating System for Which Software is Written

The code was tested on a PC using the Windows 10 operating system and using Windows Subsystem for Linux (WSL) with the Ubuntu 18.04 LTS Linux system. Since the code does not use any specialized features, it should operate correctly under any version of Linux. It should operate under a normal Linux system or on a PC using the WSL interface and other versions of Linux.

2.8.1. Programing Language

2.9. Compiler Version

The code uses the GNU f77 Fortran compiler. Compile flags are set in a Makefile and use the "dec" feature compatibility option.

The code is invoked through the C-shell interface.

The C-shell interface calls a Perl script to run the code and to move the output files to various locations within the directory structure.

2.10. Software Limitations

There are no significant software limitations related to either data storage or computational time. The code is designed for a single processor and does not use any computational algorithms that would have merit in a parallel or multi-core/cpu implementation.

The code uses some dated legacy Fortran features that should be updated to a more modern Fortran syntax in the future.

The code has some hard-coded directory locations that, if changed, will need to be modified within the source code to match the user-selected implementation location. Some of these hard-coded locations are currently configured to reach into parallel implementations of the SNL-NJOY-2016 code and the SNL-LSL code.

2.11. Related/Auxiliary/Co-Requisite Software

The code is invoked in a script that has been tested using Perl 5, version 26.

2.12. Hardware Requirements

There are no unusual hardware requirements. The hardware should have the memory and processor speed needed to support use of the Windows 10 operating system.

2.13. List of Main References for Submission Form

The relevant references consist of the NJOY-2016 manual, the ENDF/B-VIII.0 cross section library, and the IRDFF-II dosimetry cross section library.

[1] Trkov, A., Griffin, P.J., Simakov, S.P., Greenwood, L.R., Zolotarev, K.I., Capote, R., et al., "IRDFF-II: A New Neutron Metrology Library", Nuclear Data Sheets, Vol. 163, pp. 1-108, 2020.

[2] "ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data Files ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII", edited by A. Trkov, M. Herman, D.A. Brown, report CSEWG Document ENDF-102, report BNL-203218-2018-INRE, February 1, 2018. Available at: https://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

[3] D.A. Brown, M.B. Chadwick, R. Capote, et al., "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," Nuclear Data Sheets, Vol. 148, pp. 1-142, February 2018.

2.14. Funding Information

C7 (NNSA Nuclear Survivability Engineering Campaign), Project 188897 $50,000, (2010-2020)
Susan Norwood, NA-115 (202-586-4779), susan.norwood@nnsa.doe.gov

2.15. Treaties/Agreements/IP Management Plans

None.

2.16. Sensitivities

None. This code is unlimited release with no distribution limitations. The source code is made available on a public Git-based code repository.

2.17. Commercialization/Distribution Plans

There are no plans for commercialization of the software. The software is to be provided to the general radiation effects community in order to improve our basic physics understanding of neutron-induced material damage.

The software will be distributed via GitHub. The tentative link for the project is:

https://github.com/pjgriff/Manipulate-2020

While pending approval for use of the open code repository, a version of the software is currently available at:

https://gitlab-ex.sandia.gov/bdhehr/Manipulate-2020

The specific license software is: BSD-3 since this provides the best permissive license for our intent.

I would like to release the code because it is of value to the general radiation effects community. Many parties are already making their own code patches to implement this data manipulation capability, e.g., the ASTM standards community is results from this code to support current standards. A general release like this is one way to focus the efforts of the international community and prevent duplicative efforts. This release will provide a framework where others can contribute their efforts to verify the software, provide validation evidence for various classes of radiation-induced damage, and expand the damage modeling.

2.18. Further Development

The data manipulation capabilities of this code are expected to be expanded to match the needs of the application community. Further development is expected and will be reflected in updates to the GitHub repository.

3. INSTALLATION

The following steps will install the code:

1. The first step in the installation is to clone the code from GitHub repository.
2. If the default directory structure is not used, then the user needs to change the hard-coded directory locations within the source code.
3. The Makefile should be used to recompile the code. This Makefile will place the executable in the proper location under the "bin" subdirectory.

4. DESCRIPTION OF STRUCTURE OF INPUT FILE

The input file consists of four input segments.

The first segment is a title card in a80 format.

The second segment is a series of control integers in 19I2 format. Table 4-1 provides a description of the input control flags.

The third segment is a set of input descriptors that will vary based upon the control flags.

The fourth segment is a termination line that has the format " 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0". The "9" flags the end of the calculation.

Table 4-1. Control Flags for Manipulate-2020 Code

Control Flags: format 19I2
c icon(1) type of action
c = 9 end
c = 1 combine cross section elements - logic unclear, PJG 10/17/2012
c = 2 prepare component plot file format output
c = 3 display a matxsr file from njoy
c =-3 same as 3 for xxx.plt_89 file
c = 4 multiple plot file option
c = 5 sum and plot components
c =-5 perform statistical ananlysis on a series of functions
c = 6 fold source and response
c = 7 weight and plot function
c =-7 reciprocal weight and plot function
c = 8 file difference
c =-8 covariance manipulation options
c =10 interpolate matxsr file
c =11 interpolate tabulated file
c =12 expand by interpolation a tabulated file
c =13 expand an analytic function in 640 group structure
c =14 combine covariance files in LSL format (common energy structure) - NEW
c =15 extract PKA recoil spectrum for given reaction/energy - NEW
c =16 extract integrated PKA recoil spectrum for as a function of energy - NEW
c
c icon(2) input energy grid/data format
c = 0 njoy sand-ii 620/640/725/770 point neutron cross section
c (energies in ev, response data to be multiplied
c by 10**-3 to yield kerma units of mev-mb)
c = 1 j. kelly sand-ii pun spectrum format
c (default quantity differential number spectrum)
c compute iselect_material = 1 number fraction
c 2 energy fraction

Control Flags: format 19I2		
c		3 differential number fraction
c		4 differential energy fraction
c		5 integral number
c	= 2	same as 1
c	= 3	flash x-ray curr spectral input
c	= 4	list directed (plot output)
c	= 5	njoy sand-ii /770 point neutron pka recoil spectrum
c		(energies in ev, response data to be multiplied
c		by 10**-3 to kev)
c	= 6	njoy matxsr interface file - arbitrary structure
c	= 9	user defined - xxx.flux file
c	=10	640 group response structure = xxx.res
c	=11	arbitrary response structure = xxx.res
c		
c	icon(3)	display/output special option
c	= 0	no action
c	= 1	punch in damout format
c	= 2	punch in tdam format
c		
c	icon(4)	print energy order
c	= 0	punch high to low
c	= 1	punch low to high
c		
c	icon(5)	sand structure
c	= 0	640 groups - SAND-II
c	= 1	770 groups - SAND-II extended
c	= 2	89 groups - NuGET neutron
c	= 3	48 groups - NuGET gamma
c	= 5	175 group - Vitamin-J
c	= 6	725 group - IAEA
c		
c	icon(6)	inhibit renormalization
c	= 0	normal
c	= 1	response, inhibit renormalization in filein
c		
c	icon(7)	NJOY interface location
c	= 0	sync_Projects-Linux/NJOY-2016 default
c	= 1	sync_Linux/NJOY-2016 selection
c		
c	icon(9)	print inhibit
c	= 0	default print
c	=>0	inhibit print by this level

Control Flags: format 19I2		
c	< 0	enhance print (debug option)
c		
c	icon(10)	label replacement
c	= 0	no action
c	= 1	read new legend information
c		
c	icon(11)	special action
c	= 0	not used
c	= 1	on pka plot, divide entry 1 by entry 3
c		to produce average recoil energy -
c		when icon(2) = 5
c	= 2	on icon(1)=7 combine, punch plt-format
c		interface file on indicated dir:filename
c		(tbd)
c	icon(12)	reverse order of data read - only partially implemented
c	= 0	no effect
c	= 1	reverse
c	icon(13)	attenuation function
c	= 1	if equal to 1 and icon(1)=6, then
c		use new function for exponential attenuation
c		with coefficient alpha
c	= 2	if equal to 2 and icon(1)=6, then
c		use sensor self-shielding correction factor
c	icon(14)	new title
c	= 0	use first card in input stream
c	= 1	read-in new title
c		
c	icon(15)	flip order of data for punch
c	= 0	do nothing
c	+ 1	invert order
c		
c	icon(16)	re-direct to look for pka files
c	= 0	do nothing
c	= 1	look in njoy/output-pka directory
c	= 2	look in NJOY9-2012 for groupr/pka files
c		
c	icon(17)	point interpolation for grprin option
c	= 0	no, not used
c	= 1	yes, interpolate
c		
c	icon(18)	precision control for sum/difference
c	= 0	no action

Control Flags: format 19I2
c = 1 force 0.0 response for differences < 1.e-4 of maximum element
c
c icon(19) inversion of output energy order
c = 0 no change
c = 1 invert order
c = 6 njoy matxsr interface file - arbitrary structure

5. CODE EXECUTION INSTRUCTIONS

After installation, the code should be executed from the ../Manipulate-2020/input directory by invoking the C-shell script "manipulate", followed by the name of the input file. For example, for the example input file "example_NJOY_groupr_convert" the user should type "./manipulate-2020 example_NJOY_groupr_convert" in the WSL window.

6. SAMPLE APPLICATION CASES

The example input files are found in the ../Manipulate-2020/inp subdirectory. Supporting files from SNL-NJOY-2016 calculations are found in the ../Manipulate-2020/use_case_support_files subdirectory. The support files, generally, need to appear in the associated NJOY-2016 file system subdirectory during the code execution, but they are included in the Manipulate-2020 subdirectory for archival purposes.

6.1. NJOY/GROUPR Response Extraction

Sample input file: example_NJOY_groupr_response_convert

6.1.1. Description

This "Use Case" extracts a response function from the GROUPR module output of the SNL-NJOY-2016 code. For this case to run, the input file:

As-75_SA_in_GaAs_ENDF_VIII_0_770grp_DK_NJOY2016_xsec_survey.inp

must have been run. This file examines the ^{75}As nuclear data file from the ENDF/B-VIII.0 library [ENDF8a, ENDF8b], uses the NJOY/HEATR module to calculate the various kermas for the isotope, and used the NJOY/GROUPR module rebin these response functions into the SNL-SAND-IV 770-group energy structure. This energy structure is a superset of the commonly used SAND-II fine-group energy structure.

This case will produce two files within the ../Manipulate-2020/response directory. The files will reflect the naming found in the input file and uses the reaction identifiers, 301 and 444, as the file suffix. The 301 file corresponds to the total kerma. The 444 file corresponds to the damage energy, which, for the NJOY input file, in this case corresponds to the displacement kerma. Note, this calculation uses the SNL-NJOY-2016 code and not the original NJOY-2016 code. The damage energy in the original NJOY code does not generate the displacement kerma, but, rather, produces a sharp threshold Kinchin-Pease damage energy.

In addition to the response files, a summary of the processing, and any error conditions, will be reflected in a "*.out" file found in the ../Manipulate-2020/output subdirectory.

6.1.2. Output

The only output here is the presence of the tabulated response functions in the ../Manipulate-2020/response subdirectory. Figure 1 shows a plot of the ^{75}As damage metrics, i.e., the total neutron kerma and the displacement kerma. The neutron ionizing kerma represents the difference between the total kerma and the displacement kerma. Most of the deposited energy from the neutron interactions less than ~100 keV is from low energy recoil atoms and this deposited energy goes into the displacement kerma. At higher incident neutron energies, a higher energy recoil atom is produced and more of the energy goes into ionization.

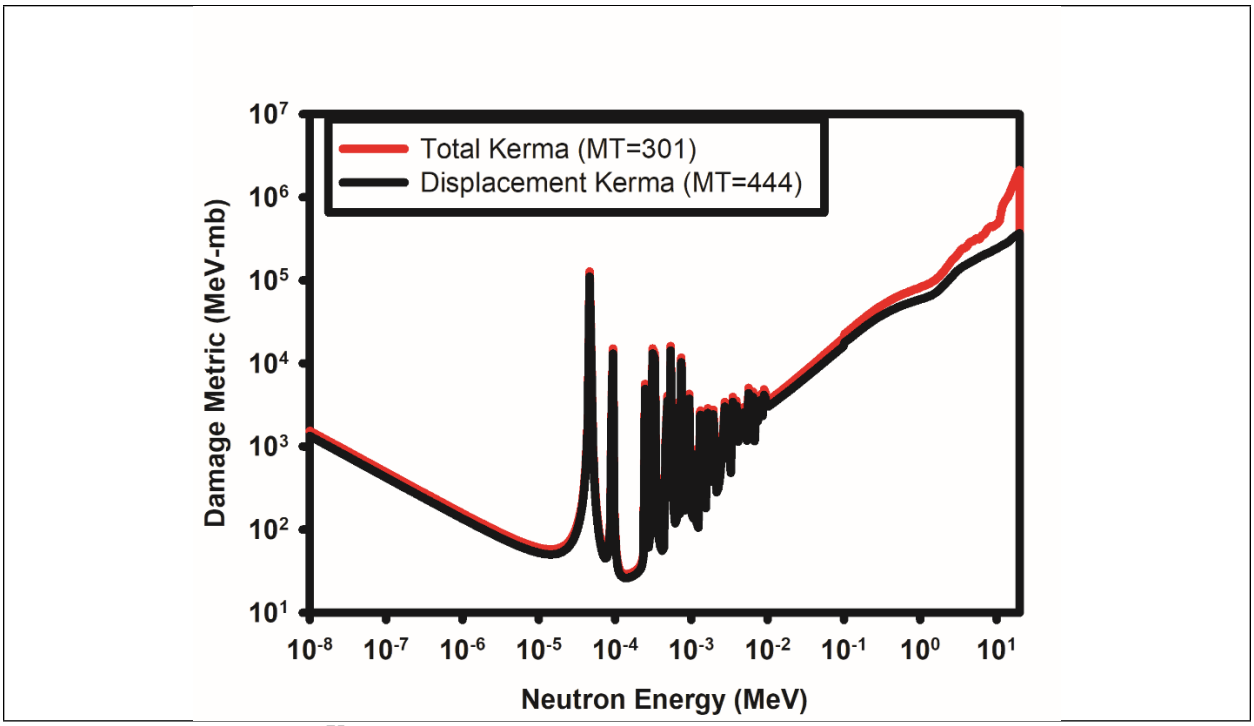


Figure 1: ^{75}As Neutron Total Kerma and Displacement Kerma Limit

6.2. Weight and Combine Response Functions

Sample input file: example_NJOY_response_combination

6.2.1. Description

This "Use Case" illustrates the weighting and combination of response files. In this simple example, we subtract the displacement kerma from the total kerma in the previous example to produce a neutron ionizing kerma.

This case will produce one file within the ../Manipulate-2020/response directory. The files will reflect the naming found in the input file and uses the suffix "IK" to indicate that is is an ionizing kerma. The input file reflects the "combination" of two responses. The first component, the total kerma, has a weighting factor of 1. The second component, the displacement kerma, has a weighting factor of -1. The result is a simple subtraction of the responses.

As in the previous example, a summary of the processing, and any error conditions, will be reflected in a "*.out" file found in the ../Manipulate-2020/output subdirectory.

6.2.2. Output

The output here is the tabular presentation of the neutron ionizing kerma that is placed in the response subdirectory. Figure 2 shows this ionizing kerma and compares it to the total and displacement

.

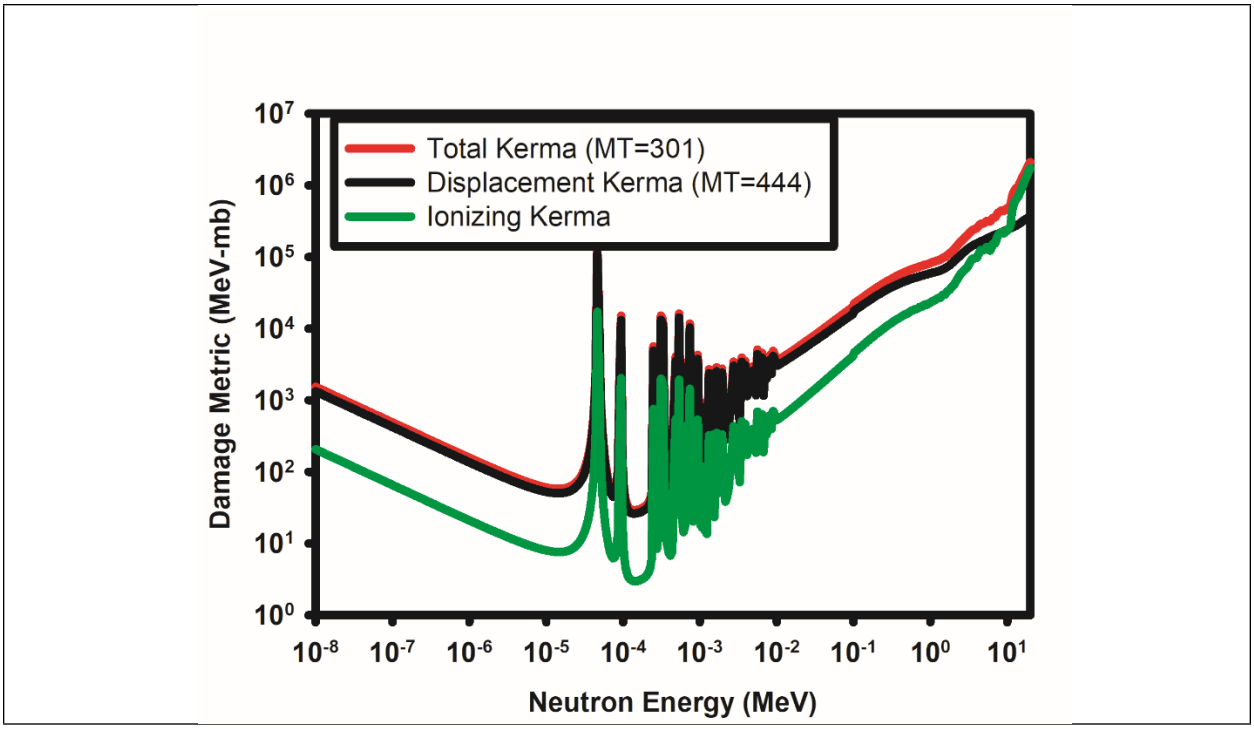


Figure 2: ^{75}As Neutron Ionizing Kerma Compared to the Neutron Total and Displacement Kermas

6.3. NJOY/GROUPR Cross Section Extraction

Sample input file: example_NJOY_groupr_xsec_convert

6.3.1. Description

This "Use Case" extracts a cross section from the GROUPR module output of the SNL-NJOY-2016 code. For this case to run, you must have previously run three SNL-NJOY-2016 input files:

Co59g_IRDFF-II_640grp_xsec.inp

Ag109g_IRDFF-II_640grp_xsec.inp

S32p_IRDFF-II_640grp_xsec.inp

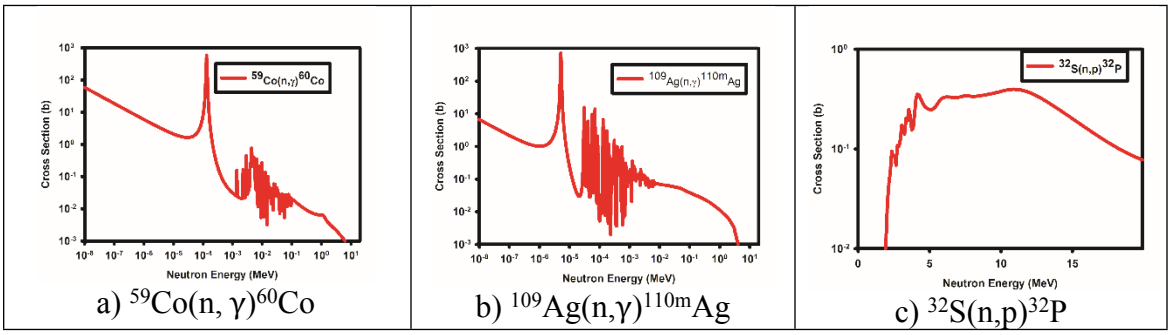
The first file generated for the ^{59}Co(n, γ)^{60}Co reaction using the IRDFF-II dosimetry cross section [IRDFF]. In this case, the cross section is found in the MF=3/MT=102 entry. The second input file generated a cross section for ^{109}Ag(n,γ)^{110m}Ag reaction using the IRDFF-II dosimetry cross section library. In this case, the cross section is found in the MF=10/MT=102 entry since the residual nucleus is a meta-stable isotope and this represents an activation product and not a MF=3 cross section. The third input file generates a cross section for the ^{32}S(n,p)^{32}P reaction using the MF=3/MT=103 component found in the IRDFF-II library.

These input files used the NJOY/GROUPR module to rebin these response functions into the SNL-SAND-II 640-group energy structure. This case will produce three files within the ../Manipulate-2020/response directory. The files will reflect the naming found in the input file and uses the reaction identifiers, 102, as the file suffix. The 102 represents the MT=102 (n,γ) reaction. The 103 represents the MT=103 (n,p) reaction.

In addition to the response files, a summary of the processing, and any error conditions, will be reflected in a "*.out" file found in the ../Manipulate-2020/output subdirectory.

6.3.2. Output

The output here is the tabular cross section that appears in the response subdirectory. Figure 3 shows the cross section for the three reactions addressed in this example.



a) $^{59}Co(n, \gamma)^{60}Co$ b) $^{109}Ag(n,\gamma)^{110m}Ag$ c) $^{32}S(n,p)^{32}P$

Figure 3: Cross Section for Example NJOY/GROUPR Extraction

6.4. NJOY/GROUPR Spectrum Extraction

Sample input file: example_NJOY_groupr_spectrum_conversion

6.4.1. Description

This "Use Case" extracts neutron spectra from the GROUPR module output of the SNL-NJOY-2016 code. For this case to run, you must have previously run two SNL-NJOY-2016 input files:

Cf252_IRDFF-II_640grp_spectrum_validation.inp

U235_IRDFF-II_640grp_spectrum_validation.inp

These files convert the NJOY/GROUPR 640-group characterization of the neutron spectra as they are found in the IRDFF-II library.

There are four segments for the Manipulate-2020 input file. Portions one and two address the ^{252}Cf(s.f.) spontaneous fission neutron spectrum. Portions three and four address the ^{235}U(nth) thermal fission spectrum. While the first and third segment do the NJOY/GROUPR extraction, the second and fourth portion of the input stream processes the spectrum and outputs the spectrum in various spectral representations. The spectrum-averaged energy is also output for inspection.

This case will produce a summary of the processing with the spectral characterization, and any error conditions, in a "*.out" file found in the ../Manipulate-2020/output subdirectory.

6.4.2. Output

The output here is the tabulation of the spectrum in multiple formats. Figure 4 shows the ^{252}Cf(s.f.) spontaneous fission neutron spectrum depicted as a differential number, differential energy, and lethargy representation. The only difference between the differential energy and lethargy representation is the use of a linear y-axis. In a lethargy representation, the use of a linear y-axis and a logarithmic energy axis means that equal areas under the curve correspond to equal probabilities for the neutron.

The ^{252}Cf(s.f.) and ^{235}U(n_{th}) fission neutron spectra have a very similar in shape. Figure 5 shows that, in a differential energy representation, the spectra can not be clearly differentiated. In the lethargy representation a small change is seen. This small change is consistent with the average neutron energy in these two spectral representations reported in the output: $\left\langle E_n^{252Cf(s.f.)} \right\rangle = 2.123615$ MeV and $\left\langle E_n^{235U(n_{th})} \right\rangle = 2.000431$ MeV.

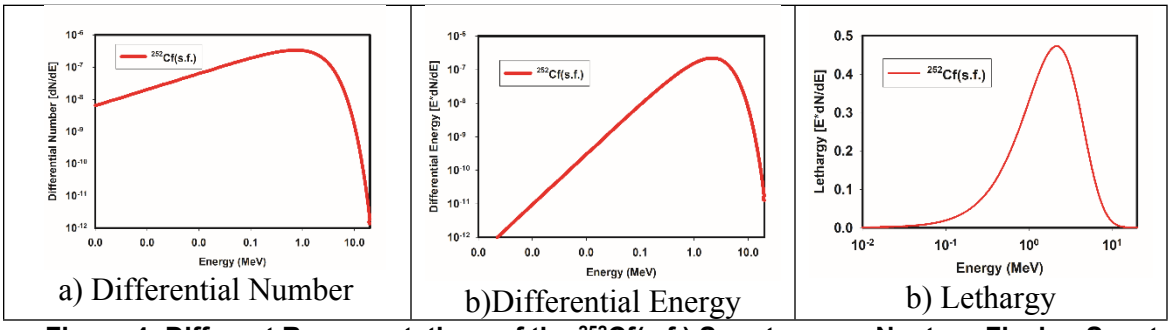


Figure 4: Different Representations of the ^{252}Cf(s.f.) Spontaneous Neutron Fission Spectrum

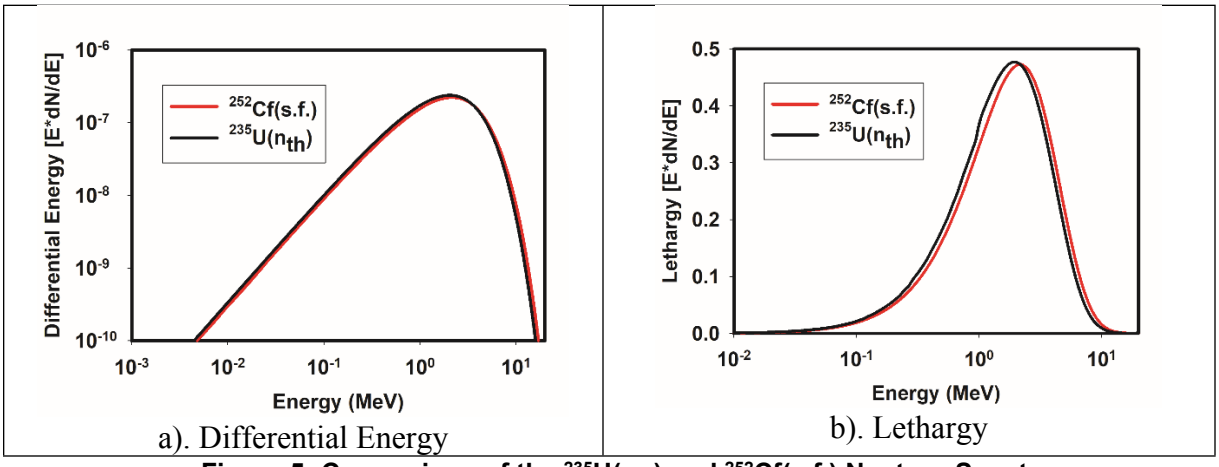


Figure 5: Comparison of the ^{235}U(n_{th}) and ^{252}Cf(s.f.) Neutron Spectra

6.5. Folding of Cross Section with Neutron Spectrum

Sample input file: example_response_fold

6.5.1. Description

This "Use Case" folds a response or cross section in with a neutron spectrum. This case uses cross sections and neutron spectra produced in the previous "use cases". The example has six segments of the calculation. The example case uses the ^{252}Cf(s.f.) spontaneous fission and the ^{235}U(n_{th}) thermal fission spectrum. These spectra are folded in with the ^{109}Ag(n,γ)^{110m}Ag, ^{59}Co(n,γ)^{60}Co, and ^{32}S(n,p)^{32}P cross sections.

This case will produce a summary of the processing with the spectral characterization, and any error conditions, in a "*.out" file found in the ../Manipulate-2020/output subdirectory.

6.5.2. Output

The output file reports spectrum-averaged cross section and the energy sensitivity regions. Table 6-1 shows a summary of the main characteristics for the two neutron spectra and three cross sections addresses in this example. These spectrum-averaged cross sections and energy response regions are similar to what is reported in ASTM E261, Standard Practice for Determining Neutron Fluence, Fluence Rate, and Spectra by Radioactivation Techniques [ASTM261], for the $^{32}S(n,p)^{32}P$ reactions. This information is also reported in the precision and bias section of ASTM E265 Standard Test Method for Measuring Reaction Rates and Fast-Neutron Fluences by Radioactivation of Sulfur-32 [ASTM265].

Table 6-1. Summary Characteristic of Spectrum/Cross Section Folding

Cross Section	Neutron Spectrum	<σ> (mb)	Response Sensitivity Energy Limits (MeV)		
			5%	50%	95%
$^{59}Co(n,\gamma)^{60}Co$	$^{252}Cf(s.f.)$	4.864277	0.04768145	0.8829955	3.446157
	$^{235}U(n_{th})$	5.026129	0.04544459	0.8577079	3.286839
$^{109}Ag(n,\gamma)^{110m}Ag$	$^{252}Cf(s.f.)$	9.34751	0.07278118	0.7176283	2.615176
	$^{235}U(n_{th})$	9.739893	0.07204609	0.7047761	2.556543
$^{32}S(n,p)^{32}P$	$^{252}Cf(s.f.)$	73.99146	2.260848	4.024577	7.734848
	$^{235}U(n_{th})$	66.82598	2.235097	3.917196	7.298408

6.6. Validate Positive Definite Attribute for the Cross Section Covariance Matrix

Sample input file: example_cross_section_covariance_verification

6.6.1. Description

This "Use Case" verifies that the cross section covariance matrix is positive semi-definite, i.e., that it does not have negative eigenvalues. Since the Manipulate-2010 code routinely checks the input file for the required mathematical properties, the easiest way to verify this is to examine the eigenvalues and to visually inspect the correlation matrix.

This case depends having run the SNL-NJOY-2016 code to extract the lsl-format covariance files. This requires that you have previously run the following NJOY-2016 cases:

Co59_ng_IRDFF-II_cor.inp

Ag109_ng_IRDFF-II_cor.inp

S32_np_IRDFF-II_cor.inp

This case will produce a summary of the processing with the spectral characterization, and any error conditions, in a "*.out" file found in the ../Manipulate-2020/output subdirectory.

6.6.2. Output

The output file report provides the eigenvalues and eigenvectors for the covariance matrix. Table 6-2 summarizes the eigenvalues obtained for the three dosimetry reactions addressed in this example set.

Table 6-2. Eigenvalues for Representative Dosimetry Cross Sections

Cross Section	Eigenvalues
$^{59}Co(n,\gamma)^{60}Co$	3.188861 0.2093912 0.6967719 0.8649985 0.9670087 0.500000 0.7999997 0.9729697 0.9000000 0.8999999
$^{109}Ag(n,\gamma)^{110m}Ag$	1.650150 0.3700236 1.097767 0.9657941 0.9778988 0.9821049 0.9854667 0.9950126 0.9937788 0.9899527 0.9920523 1.147018 0.8893262 0.9636558
$^{32}S(n,p)^{32}P$	13.95432 9.689728 6.911028 4.000117 1.946010 1.302666 1.249709 1.169561 1.231581 1.096308 0.9223984 0.7239132 0.5475745 0.6180022 0.4965166 0.1028905 0.4340180 0.2553883 0.3690853 0.3335642 0.2960616 0.3153051 0.7237343E-2 0.3198490E-2 0.3050713E-2 0.2880561E-2 0.1487948E-2 0.2106898E-2 0.2367189E-2 0.2635556E-2 0.2472797E-2 0.2558193E-2 0.9133368E-3 0.5724487E-3 0.4116856E-3 0.3343157E-6 0.3516820E-3 0.5826211E-4 0.2939752E-3 0.2508267E-3 0.2651053E-3 0.1056020E-3 0.2343758E-3 0.1228880E-3 0.1795922E-3 0.2119063E-3 0.1378094E-3 0.1313290E-3 1.000000

6.7. Cross Section Correlation Matrix Conversion for Plotting Interface

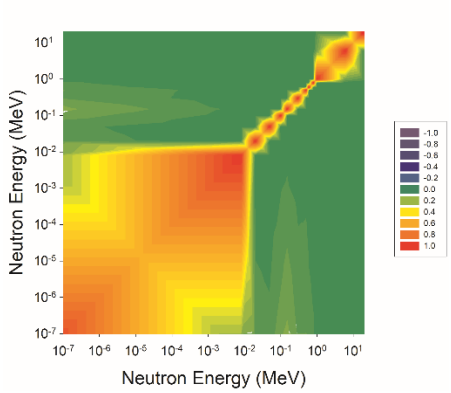
Sample input file: example_cross_section_covariance_plot_interface

6.7.1. Description

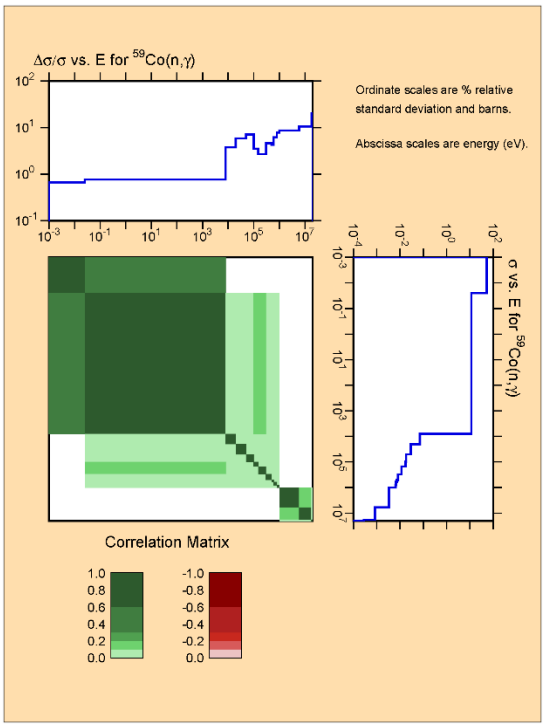
This "Use Case" verifies that examines the cross section covariance matrix in more detail by breaking it into the energy-dependent standard deviations and the energy-dependent correlation matrix. While the covariance matrix is hard to evaluate, these two derivative quantities can be plotted and visually inspected for consistency with expectations.

6.7.2. Output

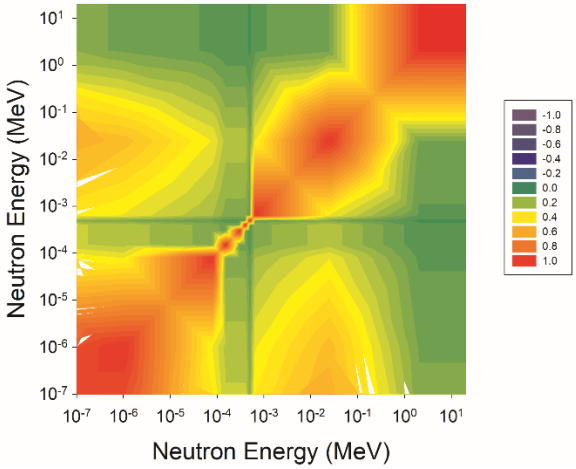
This calculation places into the output directory files that extract the energy-dependent standard deviations and the energy-dependent correlation matrix. These extracted components can be graphically depicted using commercial plotting codes. Figure 6 shows the energy-dependent correlation matrices for these reactions and compares them to the direct NJOY output for these reactions. Figure 7 shows the energy-dependent standard deviations for the three example dosimetry reactions, in the form of a percentage of the cross section.



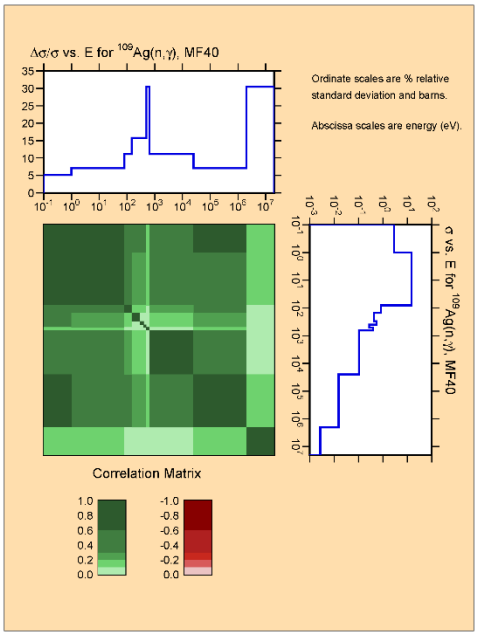
a). Manipulate-2020 $^{59}Co(n, \gamma)^{60}Co$



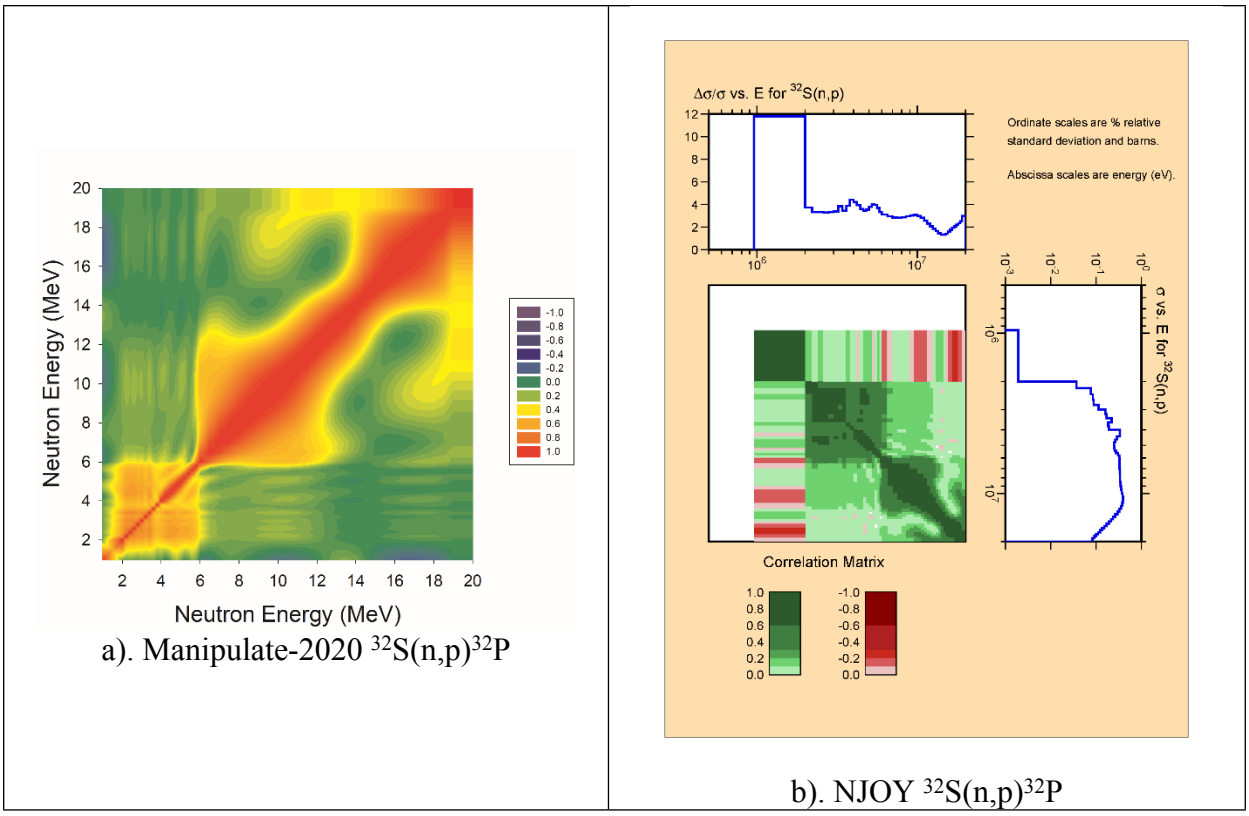
b). NJOY $^{59}Co(n, \gamma)^{60}Co$



a). Manipulate-2020 $^{109}Ag(n,\gamma)^{110m}Ag$



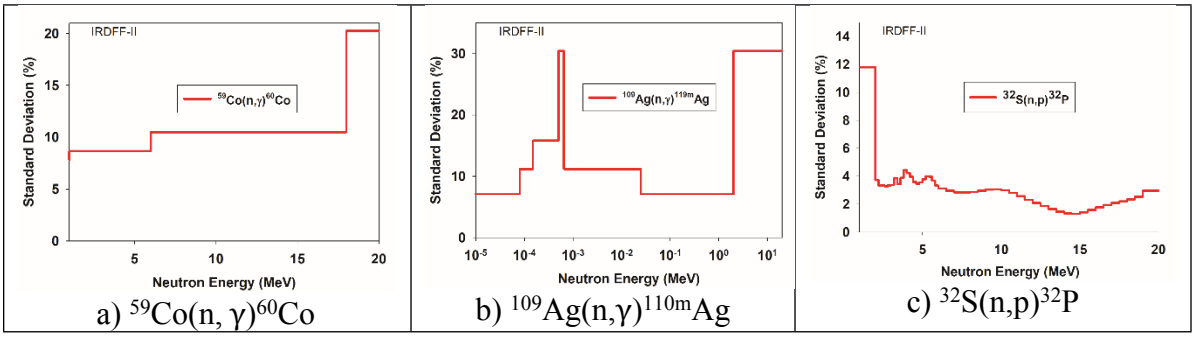
b). NJOY $^{109}Ag(n,\gamma)^{110m}Ag$



a). Manipulate-2020 $^{32}S(n,p)^{32}P$

b). NJOY $^{32}S(n,p)^{32}P$

Figure 6: Correlation Matrix for Example Dosimetry Cross Sections and a Comparison with the NJOY Output



a) $^{59}Co(n,\gamma)^{60}Co$ b) $^{109}Ag(n,\gamma)^{110m}Ag$ c) $^{32}S(n,p)^{32}P$

Figure 7: Standard Deviation for Example Dosimetry Cross Sections

6.8. Enforce Positive Definite Attribute and Unit Normalization for the Neutron Spectrum Covariance Matrix

Sample input file: example_benchmark_spectra_covariance_verification

6.8.1. Description

This "Use Case" verifies that

6.8.2. Output

The output

6.9. Spectrum Correlation Matrix Conversion for Plotting Interface

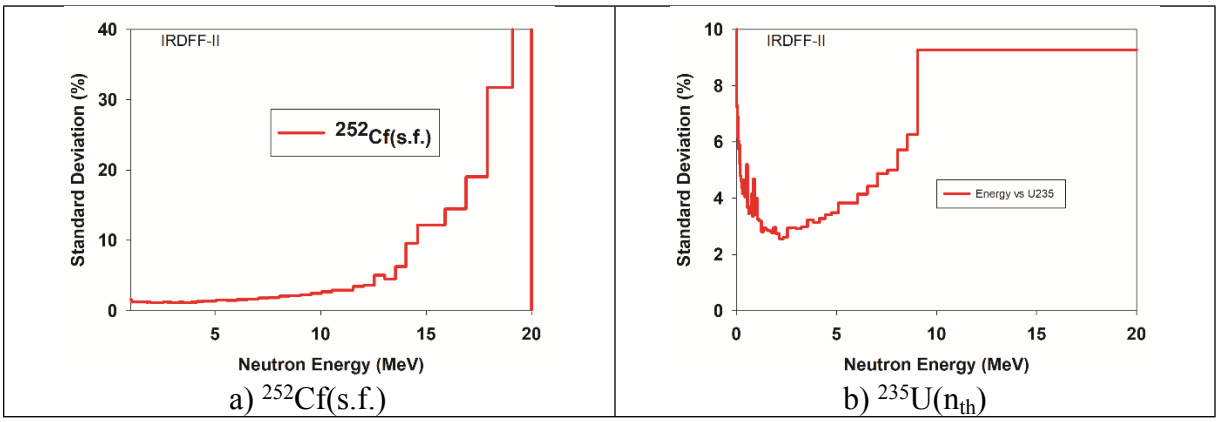
Sample input file: example_benchmark_spectra_covariance_plot_interface

6.9.1. Description

This "Use Case" verifies that

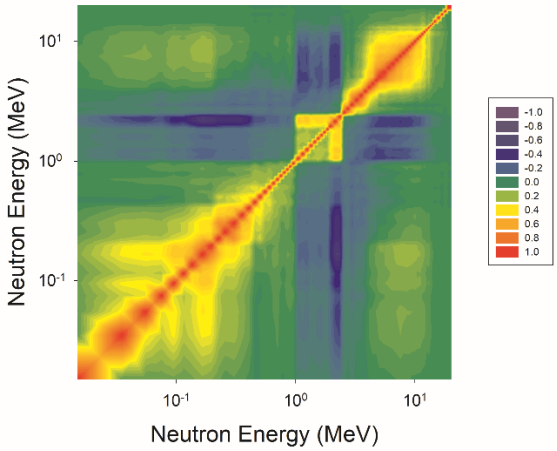
6.9.2. Output

The output

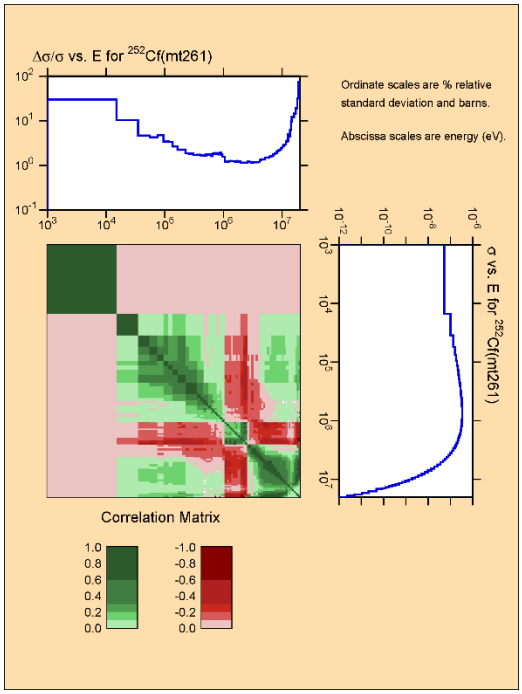


a) ^{252}Cf(s.f.) b) ^{235}U(n_{th})

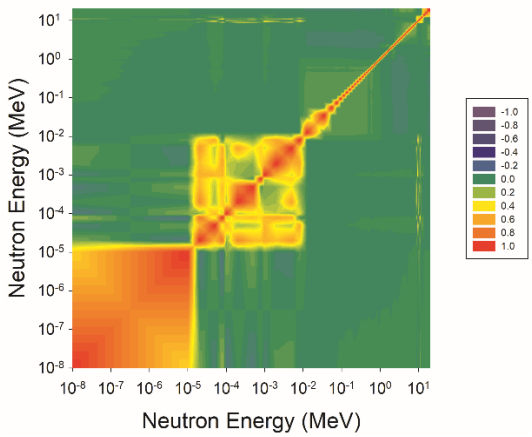
Figure 8: Standard Deviation for Benchmark Field Neutron Spectra



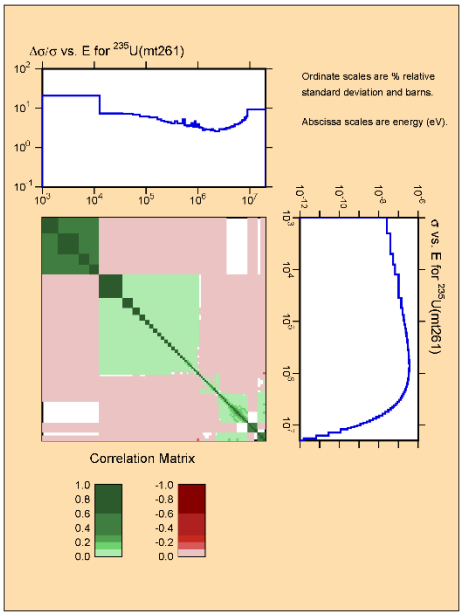
a). Manipulate-2020 ^{252}Cf(s.f.)



b). NJOY ^{252}Cf(s.f.)



a). Manipulate-2020 ^{235}U(n_{th})



b). NJOY ^{235}U(n_{th})

Figure 9: Correlation Matrix for Example Neutron Benchmark Fields and a Comparison with the NJOY Output

6.10. Spectrum Uncertainty in Spectrum-Averaged Response

Sample input file: example_spct_unc_spectrum_averaged_response

6.10.1. Description

This "Use Case" provides the uncertainty component due to the knowledge of the neutron spectrum as propagated into the spectrum-averaged response. This calculation repeats the spectrum folding using the fine 640-group representation of the response function and neutron spectrum before it does the uncertainty propagation. That initial step is performed so that the user can inspect the variation between the fine-grouped spectrum-averaged response and the spectrum-averaged response that is computed using the energy grid used for the characterization of the neutron spectrum covariance. Any big differences here may flag an issue related to the adequacy of the energy grid used in the covariance matrix for the purpose of this assessment of the spectral uncertainty contribution.

6.10.2. Output

The output file has 12 segments. There is data for the two neutron benchmark spectra; the three dosimetry cross sections which function as response functions; and two different analysis modes. As detailed in Section 6.10.1, the output listing provides the spectrum-averaged response when the fine group representation is used. The second portion of each segment provides the spectrum contribution to the uncertainty. Table 6.3 summarizes the results. In this case, the covariance representation is adequate for the intended uncertainty calculations, but the fine-group spectrum-averaged response should be used in any analysis.

Table 6-3. Summary of Spectrum Uncertainty Characteristic of Spectrum/Cross Section Folding

Cross Section	Neutron Spectrum	<σ> (mb) [640-grp]	<σ> (mb) [cov-grp]	Spct. Unc. %
$^{59}Co(n,\gamma)^{60}Co$	$^{252}Cf(s.f.)$	4.864277	5.171	2.471
	$^{235}U(n_{th})$	5.026129	4.9889	0.7529
$^{109}Ag(n,\gamma)^{110m}Ag$	$^{252}Cf(s.f.)$	9.34751	9.280	0.5645
	$^{235}U(n_{th})$	9.739893	9.6348	0.7875
$^{32}S(n,p)^{32}P$	$^{252}Cf(s.f.)$	73.99146	75.171	0.7412
	$^{235}U(n_{th})$	66.82598	67.909	1.156

6.11. Cross Section Uncertainty in Spectrum-Averaged Response

Sample input file: example_xsec_unc_spectrum_averaged_response

6.11.1. Description

This "Use Case" provides the uncertainty component due to the knowledge of the response function as propagated into the spectrum-averaged response. This calculation repeats the spectrum folding using the fine 640-group representation of the response and neutron spectrum before it does the uncertainty propagation. That initial step is performed so that the user can inspect the variation between the fine-grouped spectrum-averaged response and the spectrum-averaged response that is

computed using the energy grid used for the characterization of the response covariance. Any big differences here may flag an issue related to the adequacy of the energy grid used in the response covariance matrix for the purpose of this assessment of the uncertainty contribution.

6.11.2. Output

The output file has 12 segments. There is data for the two neutron benchmark spectra; the three dosimetry cross sections; and two different analysis modes. As detailed in Section 6.11.1, the output listing provides the spectrum-averaged response when the fine group representation is used. The second portion of each segment provides the response contribution to the uncertainty. Table 6.3 summarizes the results. In this case, the response function was also identified in a fine 640-group representation, so the fine-group spectrum-averaged response should be identical to the spectrum-averaged response in the second part of each calculation segment.

For these well characterized benchmark neutron fields, comparison with the data in Table 6-3 indicates that the response uncertainty is seen to larger than is the spectral uncertainty component.

Table 6-4. Summary of Response Uncertainty Characteristic of Spectrum/Cross Section Folding

Response / Cross Section	Neutron Spectrum	<σ> [640-grp]	Resp. Unc. %
$^{59}Co(n,\gamma)^{60}Co$	^{252}Cf(s.f.)	4.864277	4.078
	$^{235}U(n_{th})$	5.026129	3.996
$^{109}Ag(n,\gamma)^{110m}Ag$	^{252}Cf(s.f.)	9.34751	7.554
	$^{235}U(n_{th})$	9.739893	7.476
$^{32}S(n,p)^{32}P$	^{252}Cf(s.f.)	73.99146	2.484
	$^{235}U(n_{th})$	66.82598	2.534

7. CONCLUSION

This document documents the input structure for the Manipulate-2020 code and provides examples of nuclear data "manipulation". These examples map into work that applies this code to applications of interest to the ASTM standard community and to the IAEA nuclear data community. These examples can be used as stencils for user applications. This documentation is sufficient, once NNSA concurrence is obtained, to place the code within the open GitHub repository system. The nuclear data community can then use this code to reproduce analysis that has been reported in ASTM standards in in IAEA supporting documentation, e.g. the IRDFF-II library release.

REFERENCES

[ASTM1855] ASTM E1855-20, Standard Test Method for Use of 2N2222A Silicon Bipolar Transistors as Neutron Spectrum Sensors and Displacement Damage Monitors, Annual Book of ASTM Standards, Vol. 12.02, ASTM International, West Conshohocken, PA, 2020.

[ASTM261] ASTM E261-20, Standard Practice for Determining Neutron Fluence, Fluence Rate, and Spectra by Radioactivation Techniques, Annual Book of ASTM Standards, Vol. 12.02, ASTM International, West Conshohocken, PA, 2020.

[ASTM265] ASTM E265-20, Standard Test Method for Measuring Reaction Rates and Fast-Neutron Fluences by Radioactivation of Sulfur-32, Annual Book of ASTM Standards, Vol. 12.02, ASTM International, West Conshohocken, PA, 2020.

[IRDFF] Trkov, A., Griffin, P.J., Simakov, S.P., Greenwood, L.R., Zolotarev, K.I., Capote, R., et al., "IRDFF-II: A New Neutron Metrology Library", Nuclear Data Sheets, Vol. 163, pp. 1-108, 2020.

[ENDF] "ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data Files ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII", edited by A. Trkov, M. Herman, D.A. Brown, report CSEWG Document ENDF-102, report BNL-203218-2018-INRE, February 1, 2018. Available at: https://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

[ENDF8a] D.A. Brown, M.B. Chadwick, R. Capote, et al., "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," Nuclear Data Sheets, Vol. 148, pp. 1-142, February 2018.

[ENDFB8b] ENDF/VI Release 8 files are available at: http;://www.nndc.bnl.gov/csewg/summary8.html

DISTRIBUTION

Email—Internal

Name	Org.	Sandia Email Address
Michael Gregson	00512	mwgregs@sandia.gov
Daniel Dorsey	00513	djdorse@sandia.gov
Patrick Griffin	01000	pjgriff@sandia.gov
J. Charles Barbour	01300	jcbarbo@sandia.gov
E. Frederick Hartman	01340	efhart@sandia.gov
Bryan Oliver	01340	bvolive@sandia.gov
Joseph Castro	01341	jpcastr@sandia.gov
Donald Bruss	01341	dbruss@sandia.gov
K. Russell DePriest	01341	krdepris@sandia.gov
Michael McLain	01343	mlmclai@sandia.gov
Jeffrey Black	01343	jefblac@sandia.gov
James Bryson	01344	jwbryso@sandia.gov
Dolores Black	01344	dablack@sandia.gov
J. Kyle McDonald	01344	jkmcdon@sandia.gov
Arlen Heger	01354	aheger@sandia.gov
Biliana Paskaleva	01356	bspaska@sandia.gov
Matthew Burger	01380	mjburge@sandia.gov
William Martin	01384	wjmarti@sandia.gov
Andrew Tonigan	01384	amtonig@sandia.gov
David Epp	01390	dsepp@sandia.gov
Edward Bielejec	01866	esbiele@sandia.gov
Rodney Keith	08841	rlkeithsandia.gov
Technical Library	01177	libref@sandia.gov

This page left blank

This page left blank

Sandia National Laboratories

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.