

TENDL-2008:

*“Consistent **T**ALYS-based **E**valuated **N**uclear
Data **L**ibrary including covariance data”*

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Abstract

This short report describes the status of the new **TENDL-2008** library (**T**ALYS-based **E**valuated **N**uclear **D**ata **L**ibrary) developed at NRG. This library consists of a set of 348 ENDF neutron data files, ACE files, plot files and processed covariance files for isotopes from ^{19}F to ^{209}Po , stable and long-lived nuclides, completely and consistently evaluated using the TALYS-1.0 nuclear reaction code package [1]. For all isotopes and incident particles, the same methodology is applied to obtain cross sections, angular distributions, double differential data, gamma production data, isomeric production cross sections covariance information. The result is a nuclear data library with mutually consistent reaction and covariance information for all isotopes.

For incident neutrons, the following sections of evaluated files are included:

- Evaluation description (MF1),
- Resonance parameters (MF2) are based on latest measurements and compilations,
- Cross sections (MF3), elastic angular distribution (MF4), double-differential and gamma production information (MF6), and isomeric production (MF8-10), are obtained from TALYS-1.0 calculations based on consistent sets of parameters,
- Covariance files for resonance parameters (MF32) are based on the latest measurements and compilations,
- Covariance files for cross sections (MF33, with cross-reaction correlation) are obtained by means of TALYS Monte Carlo calculations,
- Covariance files for elastic angular distributions (MF34, up to the 6th Legendre polynomial coefficient) are also obtained by means of TALYS Monte Carlo calculations.

This library has been checked with the CHECKR, FIZCON and PSYCHE checking programs and successfully processed with NJOY and the latest version of ERRORJ (taking into account scattering radius uncertainty and high order Legendre polynomials in MF34). For this version, no optimal agreement with experimental data has been intended (with the exception of the capture channels), at least for the fast neutron range. This will change in TENDL-2009. Nevertheless, the global quality of TALYS ensures that for several isotopes the TENDL-2008 evaluation is already superior to any existing alternative.

A similar collection of isotopic evaluations is provided for incident protons, deuterons, tritons, helions and alpha particles, though these are without covariance data. ACE libraries for all data files, for use in MCNP(X), are also provided.

All information is available on www.talys.eu and www.talys.eu/tendl-2008.

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1 Introduction

It has been advocated [2, 3] that nuclear data evaluation can be performed much more efficiently if more disciplined working methods are adopted. Basically it means that the ENDF-6 data file should not be touched manually, and is rather seen as a helpful by-product of an evaluation process. Fig.1 summarizes the approach. Once the nuclear model code and ENDF formatting code used in the evaluation process is well verified and validated, the 4 boxes labeled “Save” contain the essential information that produces a nuclear data file. All relevant experimental data for the nucleus under consideration should be readily available, as well as a file with deduced resonance parameters (and uncertainties). An input file for the nuclear model code with parameters (and uncertainties) adjusted to reproduce the available experimental data produces a complete set of nuclear reaction results. Finally, a formatting code produces the ENDF-6 data file, which is driven by a script that performs any additional actions such as copy-paste from existing data libraries or, if necessary, scientifically dubious adjustments for the sake of good performance of the data file in applications. As Fig.1 suggests, this could be done for all nuclides and the system would consist of “blind” evaluations for isotopes which are either relatively unimportant or have no experimental data available, and very detailed evaluations with fine tuned model parameters, direct inclusion of certain sets of experimental data, etc. for the important and/or well-measured nuclides. The central message is that the data library can be automatically produced from its components, and that the knowledge of the data evaluator can be preserved in a much more compact way than in an entire ENDF-6 data file.

This new approach should not be confused with “quick and dirty” or “blind automated” nuclear data production, it should rather be called “systematic evaluation”. What this approach guarantees is that all information emerging from large efforts invested in single nuclide evaluation will remain at our disposal forever: reproducibility of the evaluation process is essential, while a bare undocumented ENDF-6 file, produced by a retired evaluator, usually does not give a lot of insight. In [3] we already showed one possible reward of this approach: exact uncertainty propagation using Monte Carlo nuclear data file production and validation. In this document we deliver another one: complete nuclear data libraries including covariance data for almost the entire nuclide chart, and all projectiles.

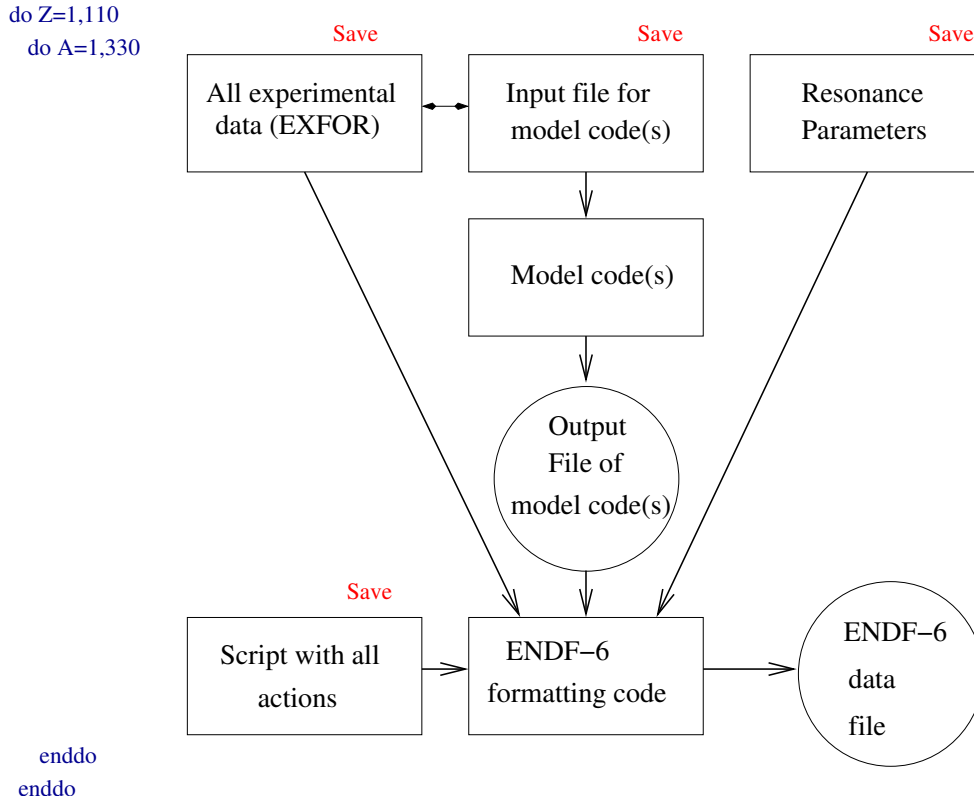


Figure 1: Flowchart of automated, reproducible evaluation process.

2 Methodology

Evaluations in the TENDL-2008 library are produced with TALYS-1.0. Various other codes developed at NRG are used for during the evaluation work:

1. Resonance range: The Reich-Moore approximation of the R-matrix theory is used to represent cross sections in the resolved resonance range. All resonance parameters are obtained from experimental data and from compilations. These resonance parameters (including the scattering radius) are adjusted to match integral measurements such as the thermal capture and elastic cross sections. The TARES code is used to convert experimental and compiled resonance information into the ENDF format.
2. Fast neutron range: All reactions (cross sections, single and double differential data, emission spectra...) are calculated with TALYS-1.0 and an adjusted set of theoretical parameters for the optical model,

the compound nucleus model, the pre-equilibrium model and nuclear structure information.

3. Covariance files: Three types of covariance files are used: MF-32 for the resonance parameters, MF-33 for cross section covariances (with cross correlations between reactions) and MF-34 for elastic angular distribution covariances in form of Legendre polynomials.
4. Formatting: All nuclear reaction information is formatted into the ENDF-6 format using the TEFAL system.
5. Checking: All files are checked for format deficiencies with the latest checking codes (CHECKR, FIZCON and PSYCHE).
6. Processing: All files are processed with NJOY to obtain energy-grouped cross sections and energy-grouped covariances.

3 Library content

3.1 Neutron sublibrary

A total number of 348 isotopes, 267 stable and 81 radioactive, are evaluated for incident neutrons in TENDL-2008. The next tables present the evaluated isotopes in TENDL-2008 (in black for stable ones and in blue for radioactive ones). Despite this large number of evaluated isotopes, no fissionable elements are included in TENDL-2008 (above Po).

Z=9	19 F									Z=25	53 Mn	54 Mn	55 Mn						
Z=10	20 Ne	21 Ne	22 Ne							Z=26	54 Fe	56 Fe	57 Fe	58 Fe					
Z=11	23 Na									Z=27	57 Co	59 Co	60 Co						
Z=12	24 Mg	25 Mg	26 Mg	27 Mg						Z=28	58 Ni	60 Ni	61 Ni	62 Ni	63 Ni	64 Ni			
Z=13	27 Al									Z=29	63 Cu	64 Cu	65 Cu	66 Cu					
Z=14	28 Si	29 Si	30 Si	31 Si	32 Si					Z=30	64 Zn	66 Zn	67 Zn	68 Zn	70 Zn				
Z=15	31 P									Z=31	69 Ga	71 Ga							
Z=16	32 S	33 S	34 S	36 S						Z=32	70 Ge	72 Ge	73 Ge	74 Ge	76 Ge				
Z=17	35 Cl	36 Cl	37 Cl							Z=33	75 As								
Z=18	36 Ar	38 Ar	39 Ar	40 Ar	41 Ar					Z=34	74 Se	76 Se	77 Se	78 Se	80 Se	82 Se			
Z=19	39 K	40 K	41 K							Z=35	79 Br	81 Br							
Z=20	40 Ca	41 Ca	42 Ca	43 Ca	44 Ca	45 Ca	46 Ca	48 Ca											
Z=21	45 Sc	46 Sc								Z=36	78 Kr	80 Kr	82 Kr	83 Kr	84 Kr	85 Kr	86 Kr		
Z=22	46 Ti	47 Ti	48 Ti	49 Ti	50 Ti					Z=37	85 Rb	87 Rb	88 Rb						
Z=23	49 V	50 V	51 V							Z=38	84 Sr	86 Sr	87 Sr	88 Sr	89 Sr	90 Sr			
Z=24	50 Cr	51 Cr	52 Cr	53 Cr	54 Cr					Z=39	89 Y	90 Y	91 Y						
Z=40	90 Zr	91 Zr	92 Zr	93 Zr	94 Zr	96 Zr													
Z=41	93 Nb	94 Nb	95 Nb																
Z=42	92 Mo	93 Mo	94 Mo	95 Mo	96 Mo	97 Mo	98 Mo	99 Mo	100 Mo										
Z=43	98 Tc	99 Tc																	
Z=44	96 Ru	98 Ru	99 Ru	100 Ru	101 Ru	102 Ru	104 Ru	105 Ru	106 Ru										
Z=45	103 Rh	104 Rh	105 Rh																

Z=46	102 Pd	104 Pd	105 Pd	106 Pd	108 Pd	110 Pd					
Z=47	107 Ag	109 Ag	111 Ag								
Z=48	106 Cd	108 Cd	109 Cd	110 Cd	111 Cd	112 Cd	113 Cd	114 Cd	116 Cd		
Z=49	113 In	115 In									
Z=50	112 Sn	114 Sn	115 Sn	116 Sn	117 Sn	118 Sn	119 Sn	120 Sn	122 Sn	124 Sn	
Z=51	121 Sb	123 Sb	124 Sb								
Z=52	120 Te	122 Te	123 Te	124 Te	125 Te	126 Te	128 Te	130 Te			
Z=53	126 I	127 I	129 I	130 I	131 I						
Z=54	124 Xe	126 Xe	128 Xe	129 Xe	130 Xe	131 Xe	132 Xe	133 Xe	134 Xe	135 Xe	136 Xe
Z=55	133 Cs	134 Cs	135 Cs	137 Cs							
Z=56	130 Ba	132 Ba	133 Ba	134 Ba	135 Ba	136 Ba	137 Ba	138 Ba	139 Ba	140 Ba	
Z=57	138 La	139 La	140 La								
Z=58	136 Ce	138 Ce	139 Ce	140 Ce	142 Ce	143 Ce	144 Ce				
Z=59	141 Pr	142 Pr	143 Pr								
Z=60	142 Nd	143 Nd	144 Nd	145 Nd	146 Nd	147 Nd	148 Nd	150 Nd			
Z=61	146 Pm	147 Pm	148 Pm	149 Pm	151 Pm						
Z=62	144 Sm	147 Sm	148 Sm	149 Sm	150 Sm	151 Sm	152 Sm	154 Sm			
Z=63	151 Eu	152 Eu	153 Eu								
Z=64	148 Gd	152 Gd	153 Gd	154 Gd	155 Gd	156 Gd	157 Gd	158 Gd	160 Gd	161 Gd	
Z=65	159 Tb										
Z=66	156 Dy	158 Dy	160 Dy	161 Dy	162 Dy	163 Dy	164 Dy	165 Dy			
Z=67	165 Ho										
Z=68	162 Er	164 Er	166 Er	167 Er	168 Er	170 Er	171 Er				
Z=69	169 Tm	171 Tm									
Z=70	168 Yb	169 Yb	170 Yb	171 Yb	172 Yb	173 Yb	174 Yb	176 Yb			
Z=71	175 Lu	176 Lu	177 Lu								
Z=72	174 Hf	176 Hf	177 Hf	178 Hf	179 Hf	180 Hf	181 Hf				
Z=73	180 Ta	181 Ta	182 Ta								
Z=74	180 W	182 W	183 W	184 W	186 W						
Z=75	184 Re	185 Re	187 Re	188 Re							
Z=76	184 Os	186 Os	187 Os	188 Os	189 Os	190 Os	191 Os	192 Os	193 Os		
Z=77	191 Ir	193 Ir	194 Ir								
Z=78	190 Pt	192 Pt	194 Pt	195 Pt	196 Pt	198 Pt					
Z=79	197 Au										
Z=80	196 Hg	198 Hg	199 Hg	200 Hg	201 Hg	202 Hg	204 Hg				
Z=81	203 Tl	204 Tl	205 Tl								
Z=82	204 Pb	206 Pb	207 Pb	208 Pb							
Z=83	209 Bi										
Z=84	209 Po										

3.1.1 Resonance range

Resonance parameters are extracted from the latest measurements (such as from the EXFOR database [4]) and from compilations (*i.e.* The Atlas of Neutron Resonances [5]). These two sources of information cover the vast majority of experimental data used for the isotopes in TENDL.

For the remaining ones (*e.g.* ^{146}Pm), hypothetical resonance levels are used with a bound level to simulate the elastic and capture cross sections not higher than 1 MeV. The parameters of these resonances are extracted from average level spacings D_0 , s -wave strength functions S_0 , radiative widths Γ_γ and scattering radius extracted from TALYS.

3.1.2 Fast neutron range

Cross sections in the fast neutron range and differential data are obtained from the TALYS-1.0 nuclear reaction code. It simulates reactions in the keV-200 MeV energy range for target nuclides of mass 12 and heavier. The following output is stored in the nuclear data file:

- Total, elastic and non-elastic cross sections,
- Elastic scattering angular distributions,
- Inelastic scattering cross sections and angular distributions to discrete states,
- Exclusive channel cross sections, *e.g.* (n,γ) , $(n,2n)$, (n,np) ..., energy and double-differential spectra,
- Gamma-ray production for discrete states and continuum,
- Isomeric and ground state cross sections,
- Residual production cross sections,
- Total particle cross sections, *e.g.* (n,xn) , (n,xp) ..., energy and double-differential spectra.

The ENDF-6 procedures to store all this information, for either neutrons or charged particles have been published in various places [6, 7, 8, 9], so we do not repeat it here.

3.1.3 Covariance information

The methods as presented in Refs. [3, 10] are used to generate covariances. Three types of covariance information are stored in our evaluations:

1. Resonance parameter covariances

From thermal energy to the end of the resonance region, covariance information is stored in the MF-32 format (resonance parameter covariances). Resonance parameter uncertainties (resonance energy and elastic and radiative widths) are obtained from the same source as resonance parameters, ensuring consistency. If no uncertainties are given in literature, default values of 0.1 % and 50 % are assumed for resonance energy and widths, respectively. Short term correlations are calculated as presented in Ref. [10]. No long-range correlations are used.

As a new feature, the scattering radius uncertainty is included in MF-32. For correct processing, the latest version of ERRORJ is necessary. If an older version is used, the scattering radius uncertainty is ignored and the elastic and total cross section uncertainties in the resonance range are underestimated.

2. Cross section covariances

In the fast neutron range, we use a Monte Carlo method in which the covariance data come from uncertainties of the nuclear model calculations. For all isotopes, the initial “best” set of results is produced by a TALYS calculation with an adjusted input parameter set. This set of results is stored in file MF-3 to MF-10. Next, for each isotope we have performed TALYS runs with random nuclear model parameters, which are used to generate uncertainties and correlations. Besides correlation within the same reaction channels, also correlation between reaction channels is included. All information on cross section covariances are stored in the MF-33 format, starting at the end of the resonance range up to 20 MeV.

3. Elastic angular distribution covariances

For the elastic angular distribution, covariance information is stored using the MF-34 format. As for the cross section covariances, we use the Monte Carlo method. In practice, the same random runs provide both information for cross section covariances and elastic angular distribution covariances. The MF-34 format makes use of Legendre polynomial coefficients to represent the covariance information. We give covariances up to the 6th Legendre polynomial coefficient.

3.2 Proton sublibrary

A total number of 344 isotopes are evaluated for incident protons up to 200 MeV in TENDL-2008. Typical contents of the proton files are

- Elastic cross section (MF-3, MT-2)
- Sum of all other cross sections (MF-3, MT-5)
- Angular distributions for elastic scattering (MF-6, MT-2)
- Residual production cross sections and energy-angle distributions of all outgoing particles lumped into MT-5 (MF-6,MT-5)

3.3 Deuteron sublibrary

A total number of 336 isotopes are evaluated for incident deuterons up to 200 MeV in TENDL-2008. Typical contents of the proton files are

- Elastic cross section (MF-3, MT-2)
- Sum of all other cross sections (MF-3, MT-5)
- Angular distributions for elastic scattering (MF-6, MT-2)
- Residual production cross sections and energy-angle distributions of all outgoing particles lumped into MT-5 (MF-6,MT-5)

3.4 Triton sublibrary

A total number of 339 isotopes are evaluated for incident tritons up to 200 MeV in TENDL-2008. Typical contents of the proton files are

- Elastic cross section (MF-3, MT-2)
- Sum of all other cross sections (MF-3, MT-5)
- Angular distributions for elastic scattering (MF-6, MT-2)
- Residual production cross sections and energy-angle distributions of all outgoing particles lumped into MT-5 (MF-6,MT-5)

3.5 Helium-3 sublibrary

A total number of 338 isotopes are evaluated for incident Helium-3 up to 200 MeV in TENDL-2008. Typical contents of the proton files are

- Elastic cross section (MF-3, MT-2)
- Sum of all other cross sections (MF-3, MT-5)
- Angular distributions for elastic scattering (MF-6, MT-2)
- Residual production cross sections and energy-angle distributions of all outgoing particles lumped into MT-5 (MF-6,MT-5)

3.6 Alpha sublibrary

A total number of 342 isotopes are evaluated for incident alphas up to 200 MeV in TENDL-2008. Typical contents of the proton files are

- Elastic cross section (MF-3, MT-2)
- Sum of all other cross sections (MF-3, MT-5)
- Angular distributions for elastic scattering (MF-6, MT-2)
- Residual production cross sections and energy-angle distributions of all outgoing particles lumped into MT-5 (MF-6,MT-5)

3.7 Photon sublibrary

A total number of 327 isotopes are evaluated for incident alphas up to 200 MeV in TENDL-2008. Typical contents of the gamma files are

- Cross sections (MF-3)
- Residual production cross sections and energy-angle distributions of all outgoing particles (MF-6)
- Absolute cross sections for production of radioactive nuclei

3.8 ACE files for MCNP use

For all particles, except photons, ACE files have been included.

3.9 x-y data tables

Besides full ENDF-6 formatted data libraries, we have also organized all our data in easy to read (or plot) x-y tables. We hope that the entire directory is self-explanatory. The contents of each file is explained at the top of that file.

4 Formatting

The data files are created automatically using our ENDF-6 format generator TEFAL, which merges all results from TALYS into a single ENDF-6 file.

5 Processing

The TENDL-2008 library was processed with NJOY-99.161 and an updated version of ERRORJ, available from G. Chiba (JAEA, Reactor Physics Analysis and Evaluation Group) or from S. Kahler (LANL, T-2) on November 2008. This latest version makes use of a format modification which allows to give the scattering radius uncertainty in MF-32 (5th line, second position), in fm.

If an older version of ERRORJ is used, the scattering radius uncertainty is ignored. For practical reasons, this format modification will be submitted to the next CSWEG format committee meeting.

The MF-34 processing has been checked for each file. ERRORJ was also modified to be able to handle 6 Legendre polynomial coefficients. The modifications are included in the latest available code version. If an older version is used, only the first Legendre polynomial coefficient can be processed. This comment is valid for any ENDF-6 file with a MF-34 section.

6 Examples

6 EXAMPLES

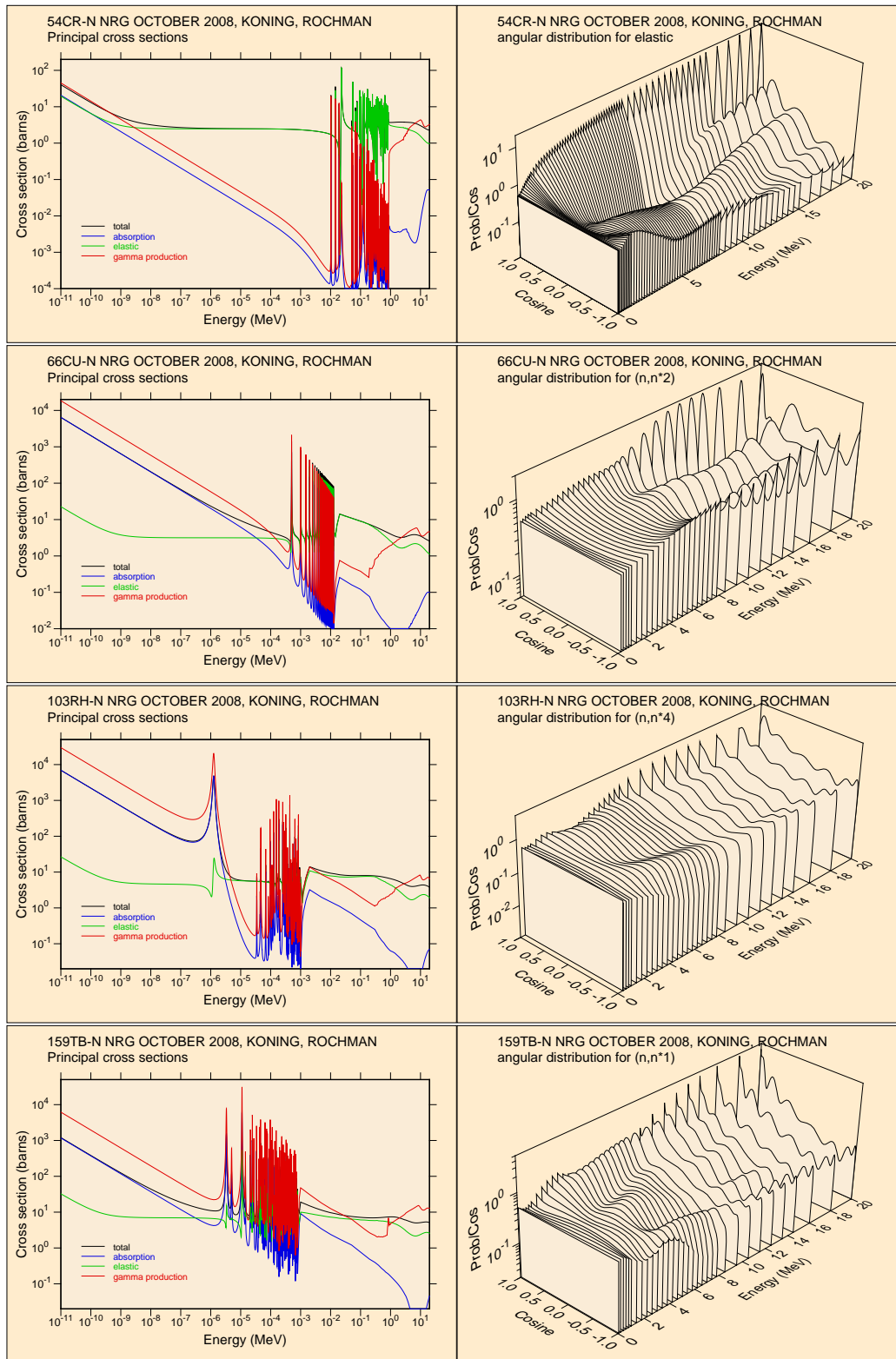


Figure 2: Cross sections and angular distributions for some isotopes after NJOY processing.

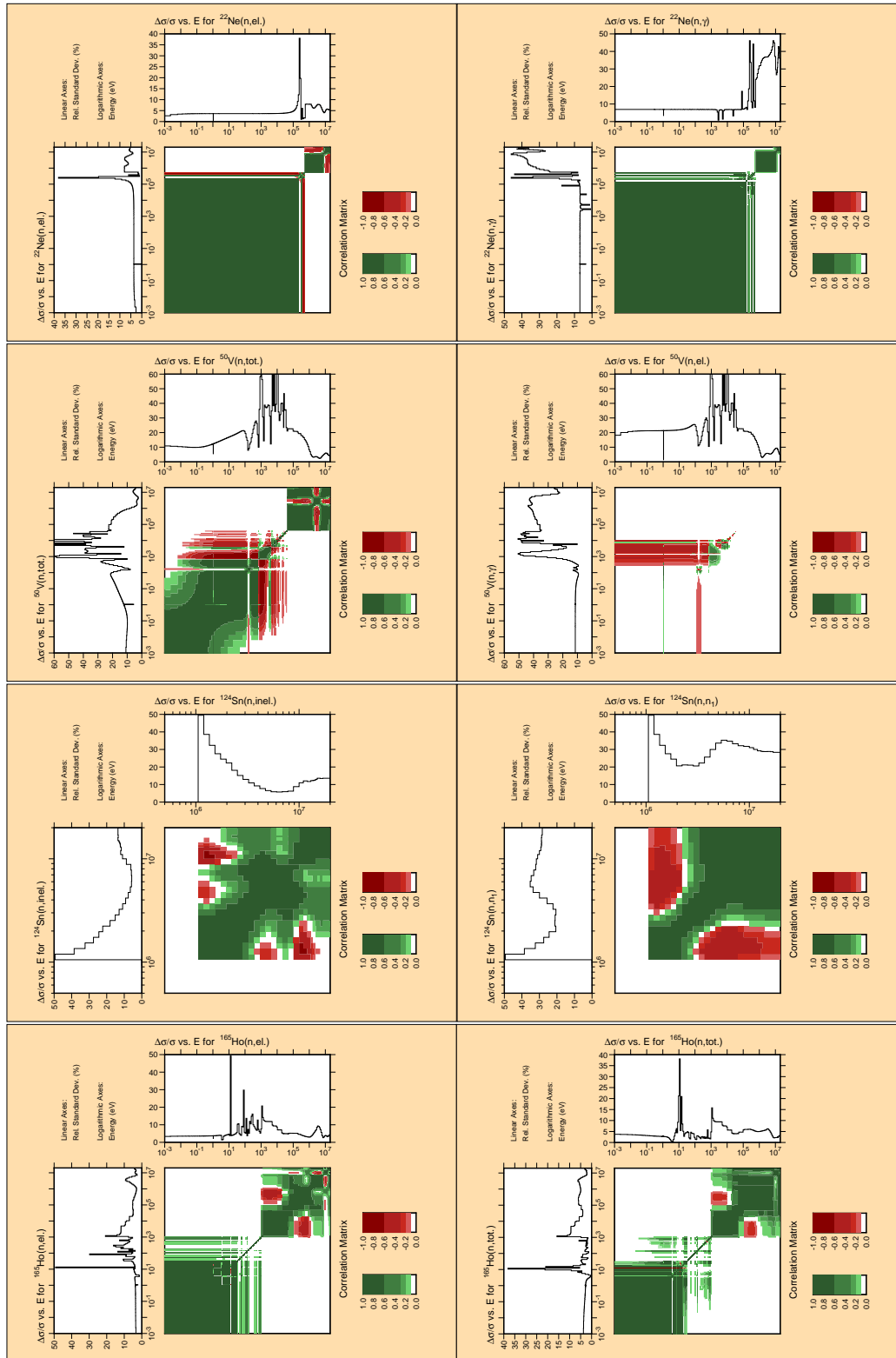


Figure 3: Cross sections uncertainties and correlations in 187 energy groups for some isotopes after NJOY processing.

7 Discussion and Outlook

As suggested in [2] and exemplified in [3] we now take a more modern approach towards nuclear data evaluation. A library is not made at a certain moment in time for one isotope, or for all isotopes of an element, but rather for the whole nuclide chart at once, whereby all specific evaluation per nuclide is kept from a previous version, or updated. We expect a large step in efficiency and quality with this approach. A few observations:

1. This is currently the only existing large scale nuclear data library for transport calculations created with one consistent approach.
2. For TENDL-2008, the evaluations for all isotopes are mutually consistent, i.e. they are equally good or equally bad, depending on your point of view. This will however change, see item 5.
3. The number of data libraries with complete covariance data is unprecedented and allows for large scale testing of covariance data in applied calculations.
4. All information belonging to an isotopic evaluation is contained in a set of resonance parameters and uncertainties and a set of Talys input parameters and uncertainties (and in the near future, a well chosen subset of EXFOR data). From this compact set of information the ENDF-6 data library is generated, i.e. the ENDF-6 data library can no longer be the starting point, since then all flexibility and incremental quality improvement would be lost.
5. From TENDL-2008 onwards, the quality of both the central value data points and the covariance matrices will improve through adjustment of TALYS input parameters per individual nuclide. Hence, we would qualify the covariance data as "reasonable" but not yet as "good". With the current systematic approach the effort to make the step from "reasonable" to "good" is however minimized as much as possible. TALYS based "real evaluations" on the isotopes of Ca, Sc, Fe, Ge, Pb and Bi, [6, 7, 8, 9, 10] as available in JEFF-3.1/3.2 β , will be included in this system and be repeated for all other non-fissile nuclides included in this set. The term "quick and "dirty" or automatic "blind" production then no longer applies. Months of effort could possibly be invested in the proper evaluation of one nuclide, this does not necessarily change from the 20th century approach. The central issue in our approach is however that after such a large single-nuclide effort the evaluation remains

completely reproducible, and that the data library can be regenerated whenever one wants, also after newer updates or corrections.

6. We would not be surprised if the isotopic evaluations from this first TENDL collection is already superior to say 40% of the isotopic evaluations in JEFF-3.1 (they surely are more complete than any of them) or other world libraries. The question is to find out for which isotopes this holds, both in the differential and integral sense. This percentage will increase rapidly if item 5. on "zeroing in on the truth" can be realized with enough momentum. For sure, TENDL-2008 contains the best open source evaluations for the natural Ne, Tm and Yb isotopes, since these exist nowhere else.
7. The statement in item 6. also entails that the current library release also throws our defense wide open: it will surely be possible to find examples where our data file is not yet in agreement with experimental data and performs worse than existing evaluations. Also, our uncertainties may be too large or too small. We do not care (in terms of reputation damage) while at the same time we do care: negative feedback is definitely welcome and will probably result in an upgraded version of the isotopic evaluation under consideration.
8. The crucial importance of an easy to use, error free EXFOR database is obvious: no unnecessary time should be wasted by setting up manual comparisons in the evaluation process with either χ^2 or plotting. WPEC SG-30 is working hard to realize this.
9. Even though we are not aware of it now, some specific ENDF-6 procedure may turn out not to be adequate in our library (e.g. a wrong or less favorable choice to store the data in a specific MF/MT combination with a certain procedure). If this is the case, it is probably inadequate in all our data files. Of course, it will then also be corrected in all evaluations simultaneously, when we run the next batch.
10. It is trivial to extend the neutron evaluations to 200 MeV, even though covariance information for high energies is poorly defined (no MF36 for spectra, though possibly MF40 for residual production). Only more computer power is required.
11. It is trivial to extend the number of isotopes for which full blown evaluations are produced to e.g. 750 (the number of isotopes in EAF), to 1250 (the number of targets with lifetime longer than 1000 sec), or 3800 (the number of targets considered in CINDER90), or more. Only more

computer power is required. Realistic physics for such exotic isotopes is of course another issue.

12. To enable an honest comparison with the exact uncertainty propagation method of [3] (now called “Total Monte Carlo”) we have included extensive covariance information: cross-reaction correlations are taken into account as well as angular distribution covariances. We are not yet aware of any processing/validation method for these extra features, but we include this information anyway.
13. If nuclear science is ever ready for a change of nuclear data format, then it should probably go through the route outlined here: since the ENDF-6 data file is no longer considered as the most basic starting point, but rather as a helpful by-product that can be processed for further use, it is at the level of processing the TALYS results or resonance data that a different choice for the format could be made. (instead of translating a mutually inconsistent set of ENDF files from different eras.)
14. For charged particles, the TENDL collection consists of data libraries for all incident light charged particles. To our knowledge, no computer code, including MCNPX, is able to use nuclear data libraries other than photons, neutrons and protons. For protons a few tens of 150 MeV or 200 MeV data files were available up to know. The current collection hopefully motivates to extend MCNPX to handle deuteron, triton, helion, and alpha particle data libraries as well.
15. In this release, the photon library does not yet contain covariance data, due to computer time constraints. In the next release, this will be included. As far as we know, no covariance data for photonuclear data files exist so far.
16. Extension of all this to actinides is definitely possible, but requires serious financial investment.

8 Acknowledgments

The authors are grateful to Go Shiba for his substantial help in the processing of this library by updating the ERRORJ code.

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