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PSI

D. Rochman

Proposition of corrections and evaluation rules for the next JEFF releases

JEFF meeting, evaluation WG, Nov. 30-Dec. 4, 2015, Institut Curie, Paris, France
JEF/DOC-1693

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Contents

- JEFF-3.2, lessons learned
- Rules for the future JEFF libraries
- JEFF-3.3 = JEFF-3.2 + covariances + simple fixes
- Conclusion

JEFF-3.2, lessons learned

- Different feedbacks were received since the release of JEFF-3.2.

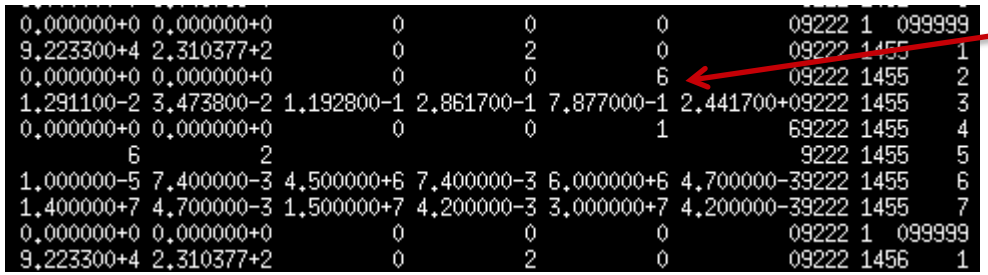
- In the following slides are given only the „*negative*“ points to be improved concerning:

  - Delayed neutrons,
  - Covariances,
  - Zr90,
  - Cu,
  - Pb, Cr52
  - U235, U238
  - Many specific MF3 MTs
  - Validation work based on Capture Resonance Integral by O. Cabellos
  - List of corrections from C. Jouanne

  - Evaluation for natural Vanadium (no slide later: shall we switch to isotopic evaluations ? Yes)

JEFF-3.2, delayed neutrons

- Issue: some actinides contain the delayed neutrons in 6 groups, other in 8 groups: inconsistency leading to difficult processing.



```
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9.223300+4 2.310377+2          0          2          0          09222 1455    1
0.000000+0 0.000000+0          0          0          6          09222 1455    2
1.291100-2 3.473800-2 1.192800-1 2.861700-1 7.877000-1 2.441700+09222 1455    3
0.000000+0 0.000000+0          0          0          1          69222 1455    4
         6          2                                            9222 1455    5
1.000000-5 7.400000-3 4.500000+6 7.400000-3 6.000000+6 4.700000-39222 1455    6
1.400000+7 4.700000-3 1.500000+7 4.200000-3 3.000000+7 4.200000-39222 1455    7
0.000000+0 0.000000+0          0          0          0          09222 1  099999
9.223300+4 2.310377+2          0          2          0          09222 1456    1
```

- 6 groups: 32 isotopes (ENDF/BVII.1: 54 JENDL-4.0: 50)
- 8 groups: 17 isotopes (ENDF/BVII.1: 0 JENDL-4.0: 0)
- 1 group: 9 isotopes (ENDF/BVII.1: 28 JENDL-4.0: 30)

- 8 groups in JEFF-3.2 including ^{235,238}U and ^{239,241}Pu

- Regarding JEFF, the CASMO manual mentions: "*No delayed neutron data has been implemented from the JEFF 3.1.1 nuclear data evaluation as the delayed neutron data is only presented in 8 delayed groups*".

- Solution: choose one group type.

JEFF-3.2, covariance

- Issue 1: JEFF-3.2 lacks complete covariances for ^{235}U, ^{239}Pu, and ^{238}U,
- Issue 2: No covariances for important isotopes: Pu, some important fission products,
- Issue 3: No covariances for fission yields.

- For the users, MF33 is more suitable, even if MF32 contains more physics,
- Above all, consistency and unicity of format needs to be mandatory.

- Solution:
  - Validate existing JEFF-3.2 covariances (real or „fake“ benchmarks)
  - If good, keep them
  - If not good, replace them with another source (ENDF/B-VII.1, JENDL-4.0, TENDL…)
  - Make use of the latest TENDL release for all the other isotopes
  - Do not use MF32, simply MF33
  - For fission yields, take GEF correlations or other sources

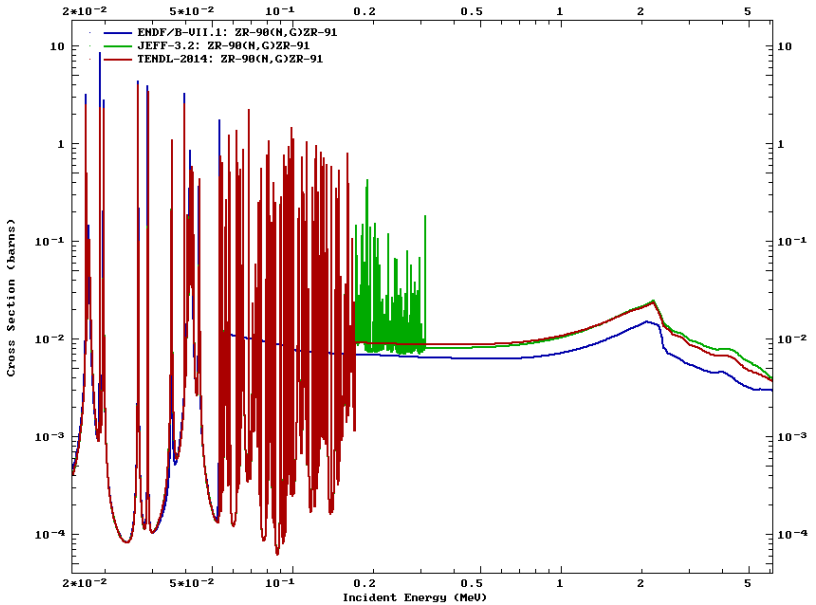
- See the discussions in the covariance WG.

JEFF-3.2, Zr-90

- In JEFF-3.2, Zr90 = TENDL-2012
- Issue: (1) As mentioned by R. Perry for Zr90: *„unphysical jump in cross-sections between the genuine resolved resonances and these statistical 'resolved' cross-sections"*

  (2) ICT-3 deteriorates compared to JEFF-3.1.2 and ENDF/B-VII.1:

	C/E, stat. unc. 40-50 pcm ICT-3 case 132	
	MONK (R. Perry)	MCNP (NEA & S. vd Marck) (same input)
ENDF/B-VII.1		1.00516
JENDL-4.0		1.00329
JEFF-3.1.1/3.1.2	0.9991	1.0044
JEFF-3.2	1.0031	1.0078
JEFF-3.2 + ^{90}Zr TENDL-2014	1.0009	



- Solution: More work needed on the benchmark and evaluation level.

JEFF-3.2, Cu evaluations

- Issue: benchmark performances, see presentations:jefdoc-1562.pdf, effdoc-1263.pdf, and effdoc-1260.pdf

Processing of the new JEFF-3.2T4…. O.Cabellos

10. Conclusions

- Processing work of new updates files has been performed.
- The impact on criticality calculations has been revised using a suite of 124 cases from ICSBEP
- In some cases differences between keff calculations and experiment increase from JEFF-3.2T3:
  - heu-met-inter-006-case2 (1.00034 -> 1.00197)
  - heu-met-inter-006-case3 (1.00372 -> 1.00545)
  - heu-met-fast-73 (1.01042 -> 1.01673)
  - ieu-met-fast-001-case3 (1.00043 -> 1.00154)
  - leu-sol-therm-007-CASE14 (0.99551 -> 0.99452)
  - u233-met-fast-004-CASE_1 (0.99924 - > 0.99856)
- An explanation of these differences could be found in the Cu63 and Cu65 evaluation in the energy range between 0.1 MeV-1.35 MeV.

  An extensive work should be performed to clarify this effect.
- For Cu63 and Cu65 some problems identified with PSYCHE code should be explained by the evaluators.
- NJOY2010/12 is required to process Cu63 and Cu65.

ENEA ITALIAN NATIONAL AGENCY FOR NEW TECHNOLOGIES, ENERGY AND SUSTAINABLE ECONOMIC DEVELOPMENT

JEFF Fusion Working Group
Paris 29-30 April, 2015

Preliminary results of Post-analysis of Copper Experiment

FPA 395-01_2.2

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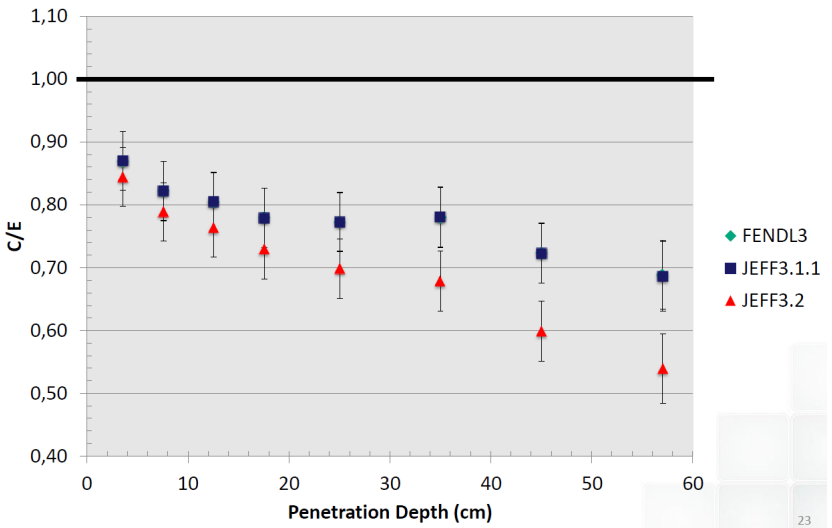
In -115 (n,n')



JEFF-3.2, Cu evaluations

- Issue: benchmark performances, see presentations:jefdoc-1562.pdf, effdoc-1263.pdf, and effdoc-1260.pdf

JEFF-3.2 COVARIANCES OF CU-63 AND CU-65 – PROBLEMS

- **No (easy) processing**
- few small negative eigenvalues, still acceptable for uncertainty analyses (~-0.002)
- **Correlation coefficients exceeding 1 ➔ UNREAL MATRICES**:
  - **Cu63**: **elastic** (up to 2.01919), MT68 (1.00037), MT69 (1.00037), MT70 (1.00037), **(n,γ)** (4.47487), (n,p) (1.08282), 104 (1.3387)
  - **Cu65**: **elastic** (up to 1.22851), MT91 (1.00051), **(n,γ)** (1.31954), (n,t) (2.55321)

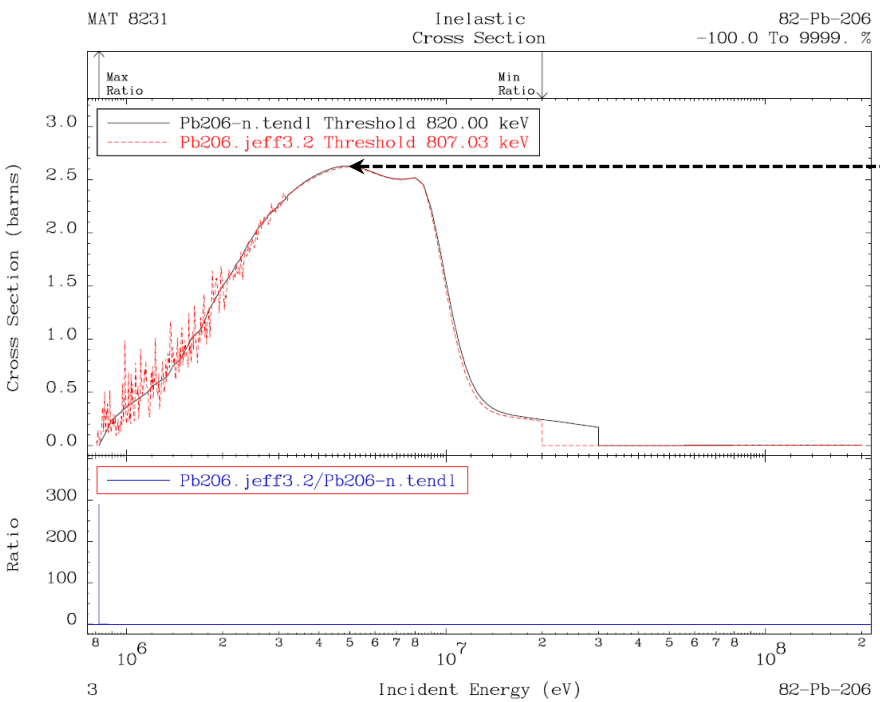
Warning: when combining covariance cross-sections and evaluations from different sources the cross-correlations between energy ranges and reactions must be carefully, consistently and integrally evaluated (reported similar problems in JENDL-4.0).

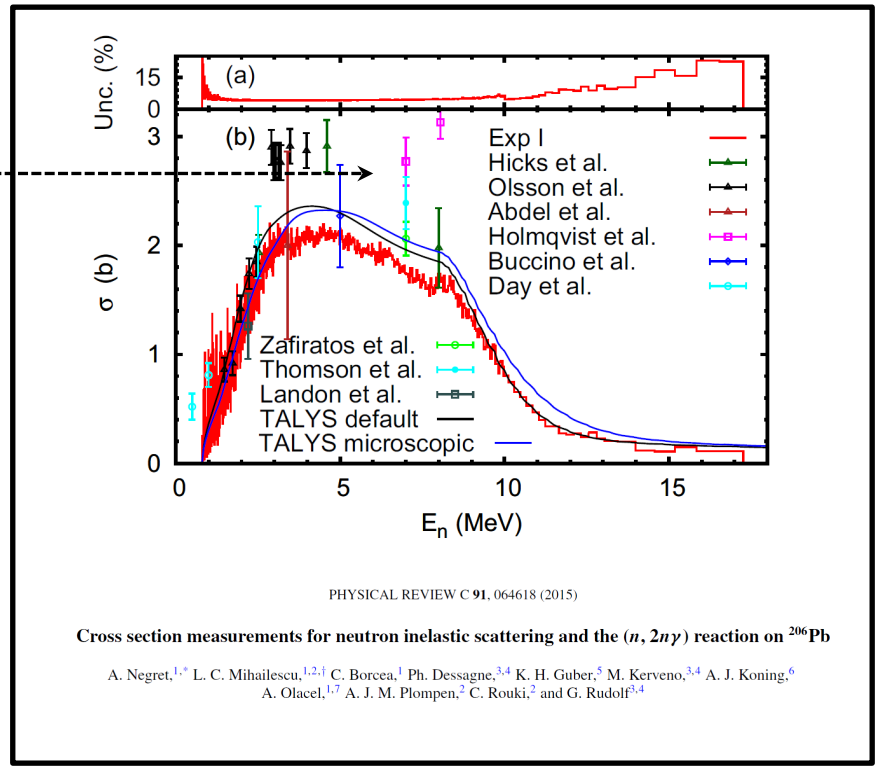
EFF Meeting, Apr. 28, 2015 15

- Solution: take a new evaluation (after checking)

JEFF-3.2, Pb isotopes

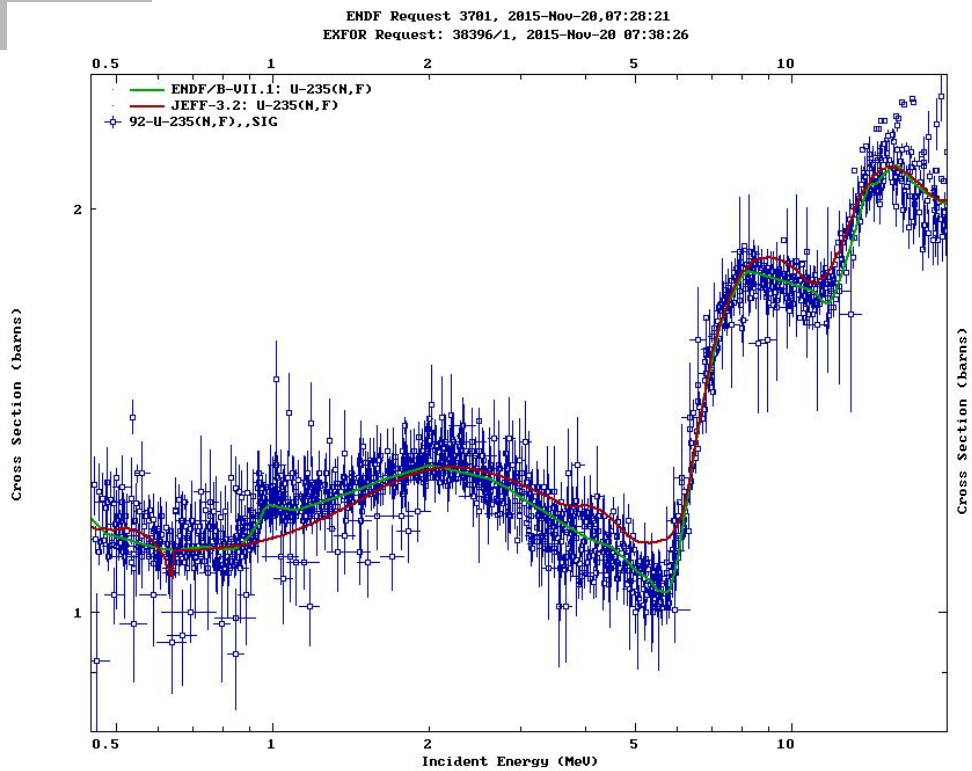
- New evaluation of Pb in JEFF-3.2, including latest (n,inl) measurements from IRMM.
- Issue: wrong procedure for the determination of the fission chamber efficiency,
- Solution: Need a new normalization with a constant factor. To be done (D. Rochman) when factor available from IRMM.

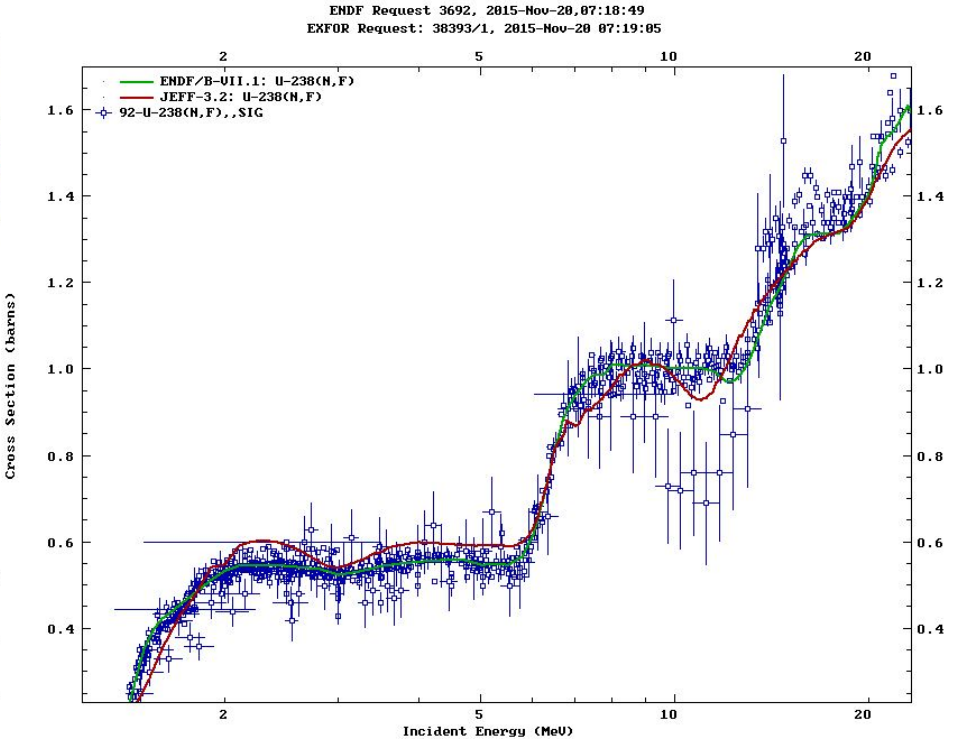




JEFF-3.2, U235, U238

- Issue: as mentioned a few times, (n,f) not matching the standards.





- Evaluations obtained from TALYS modelling.
- Solution:
  - keep as is for JEFF-3.3, re-work for JEFF-4.0)
  - adopt the best CIELO file for U-8? (IRMM preference)

JEFF-3.2, Many specific MF3 MTs

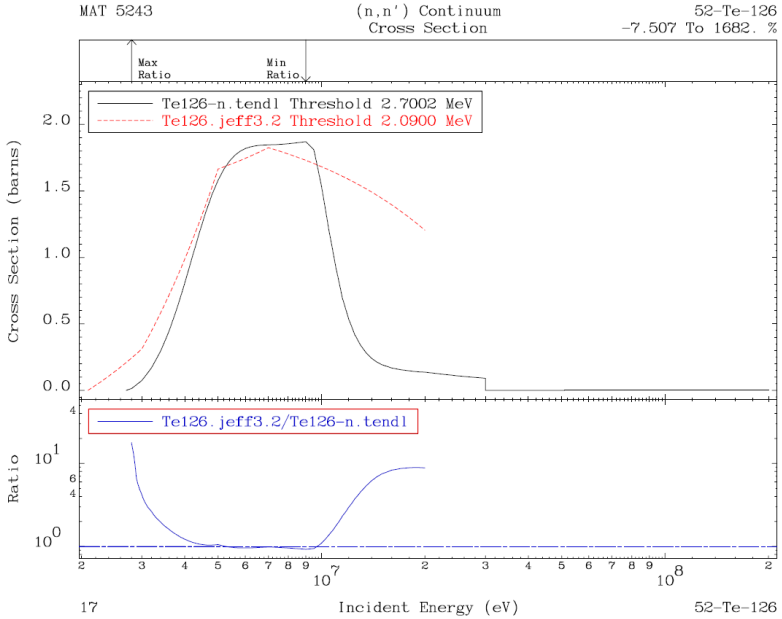
- The following isotopes present some unphysical shapes for their cross sections (MF3). Some selected cases (the best) on the next slides.

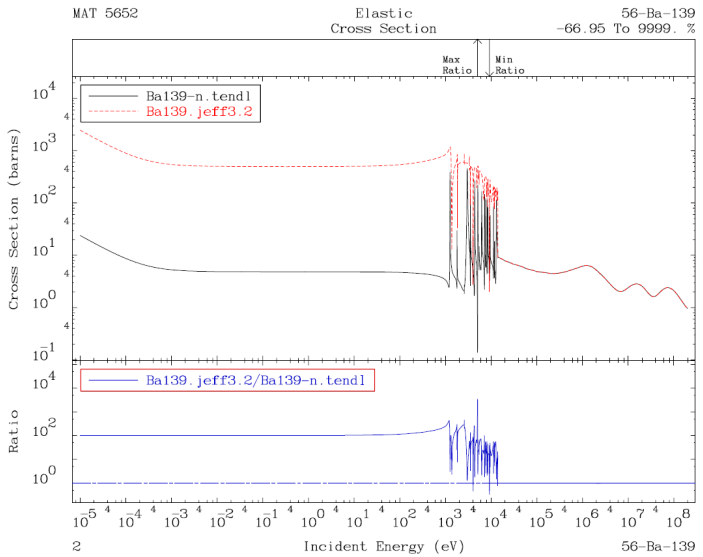
  - Unphysical MT1: ^{105}Rh
  - missing resolved resonances in MF2: ^{137}Cs, ^{124,126}Sb
  - Unphysical MT2/MT102: ^{139}Ba, ^{99}Mo, ^{100}Ru, ^{110}Pd
  - Unphysical MT16: ^{143}Nd, ^{110}Pd
  - Unphysical MT51-MT91: ^{126,128}Te, ^{150}Sm, ^{124,125,126}Sb, ^{149}Sm, ^{146}Nd, ^{135}Xe, ^{29}Si, ^{178}Hf, ^{131}Xe, ^{142}Nd
  - Missing MT51: ^{140}Ba, ^{135}Xe, ^{197}Au
  - Unexpected MT102: ^{55}Mn, ^{40}Ar, ^{177,178,179,180}Hf, ^{185}Re, ^{198,199,200,201,202}Hg, ^{130}Xe,^{142}Nd
  - Interpolation problem MT102: ^{130}I
  - Unphysical MT107: ^{241}Am

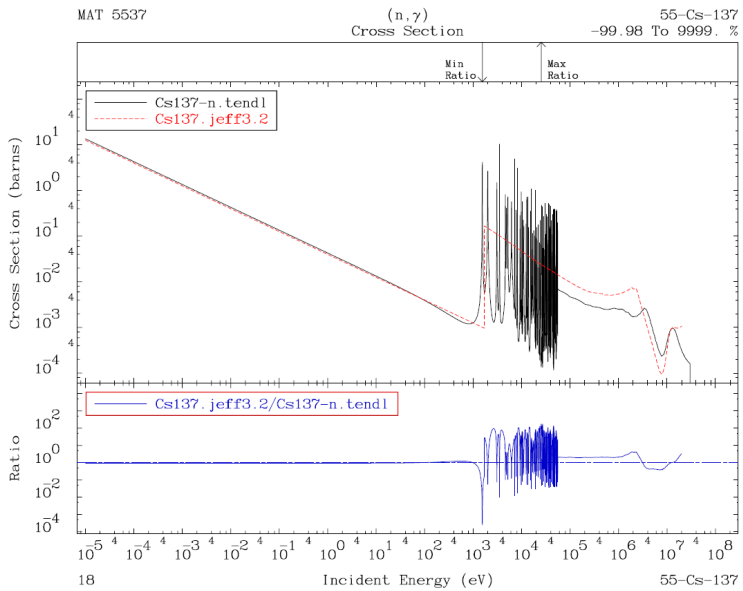
- All plots can be checked here: JEFF/TENDL ratios

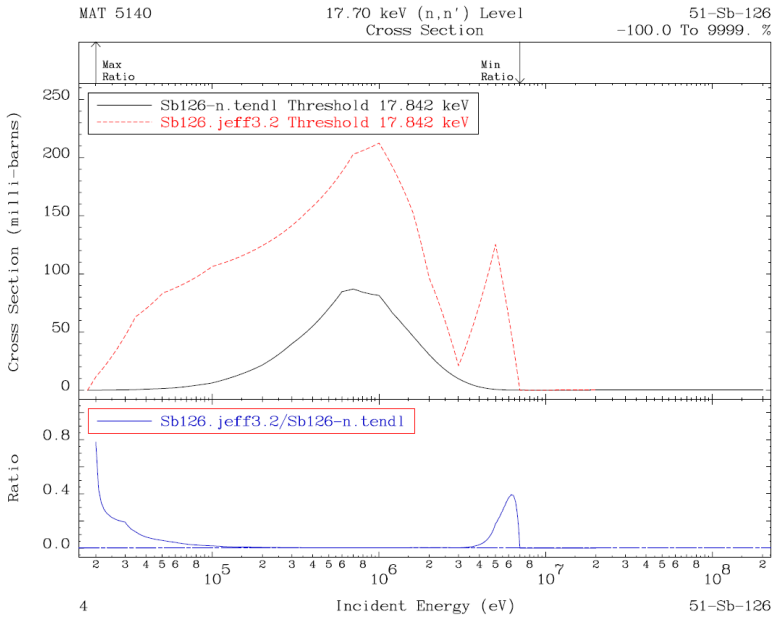
- Solution: manually correct, or take evaluations from other libraries.

JEFF-3.2, Many specific MF3 MTs

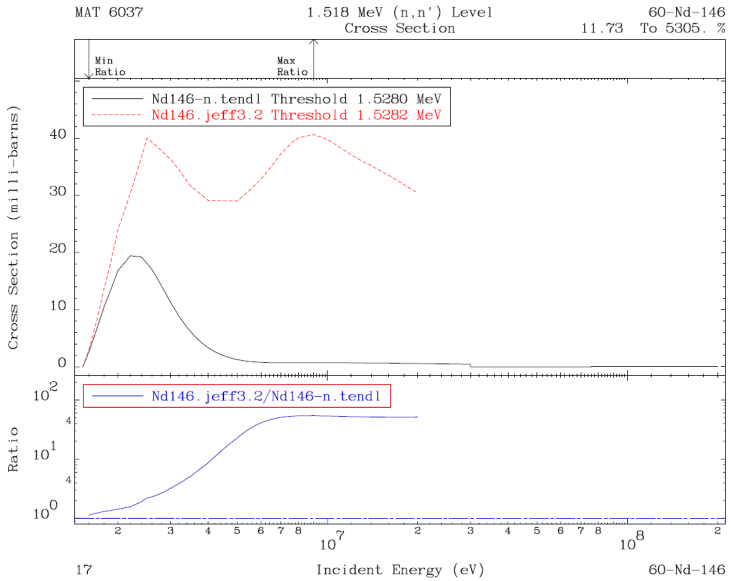


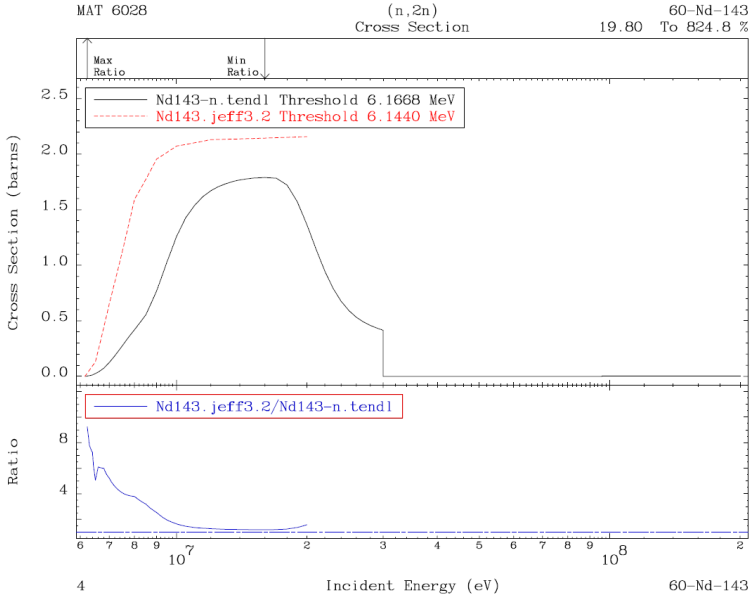


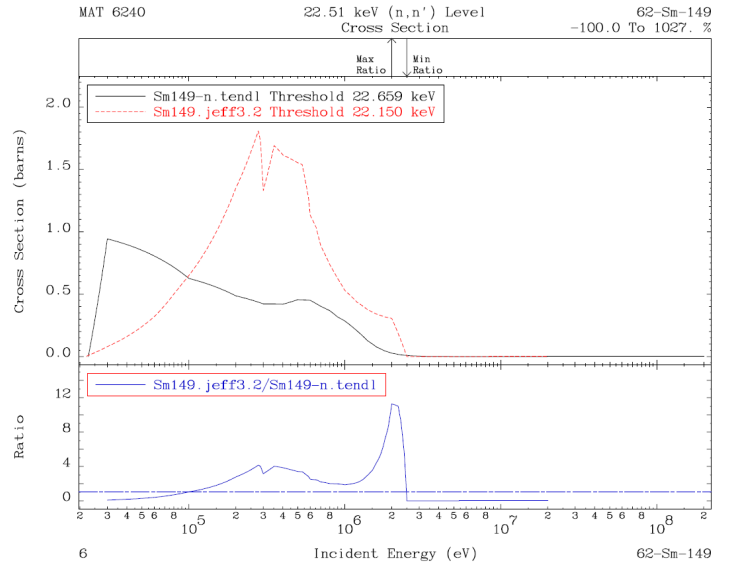


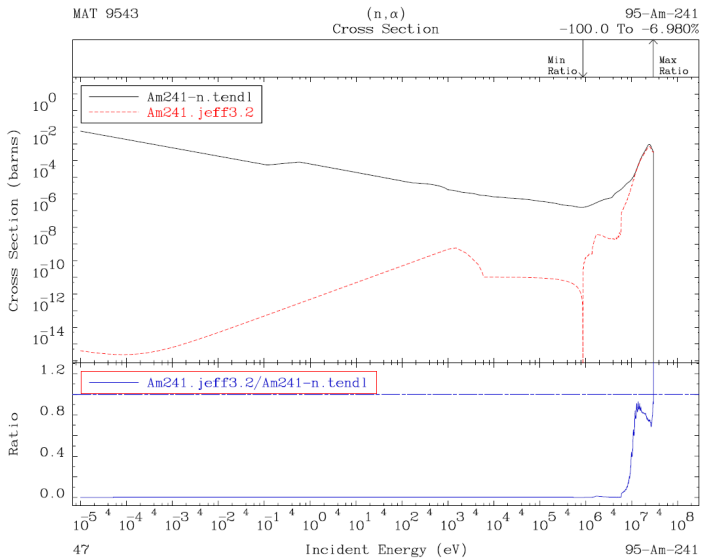


JEFF-3.2, Many specific MF3 MTs

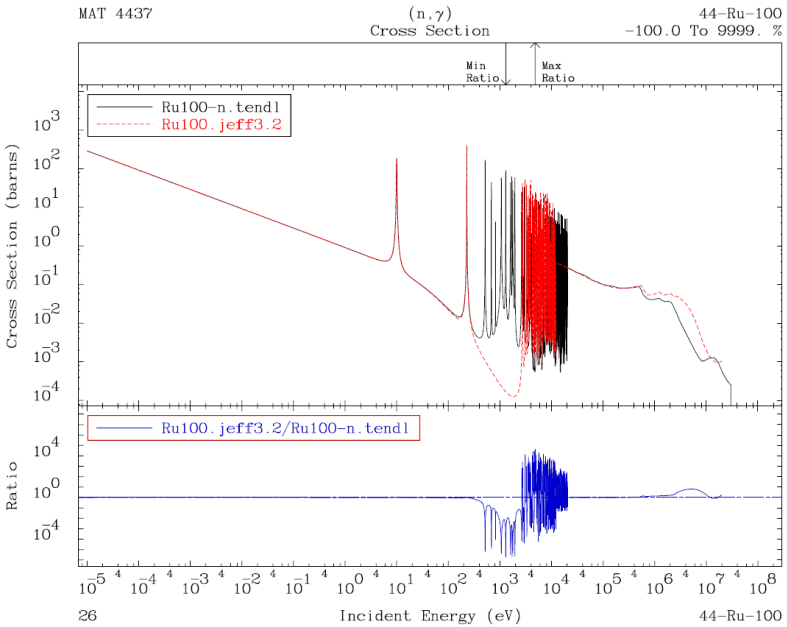


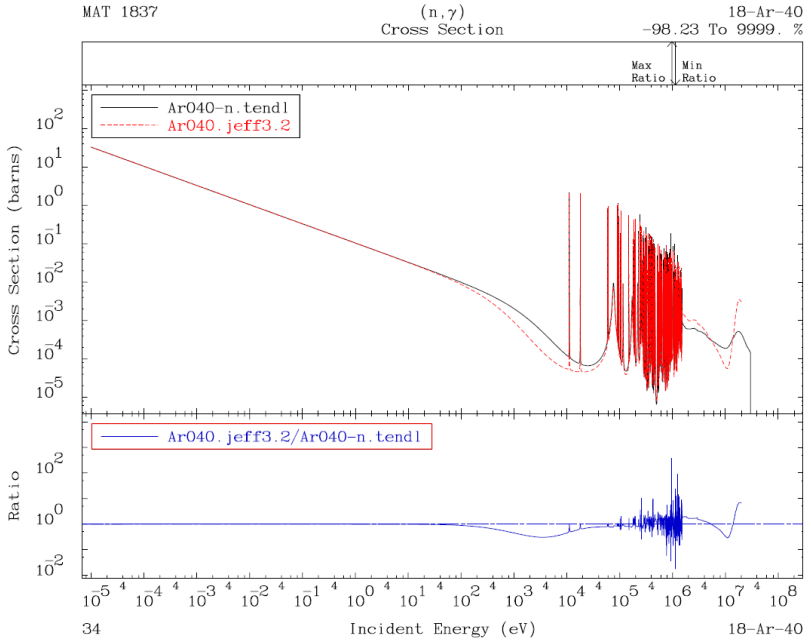


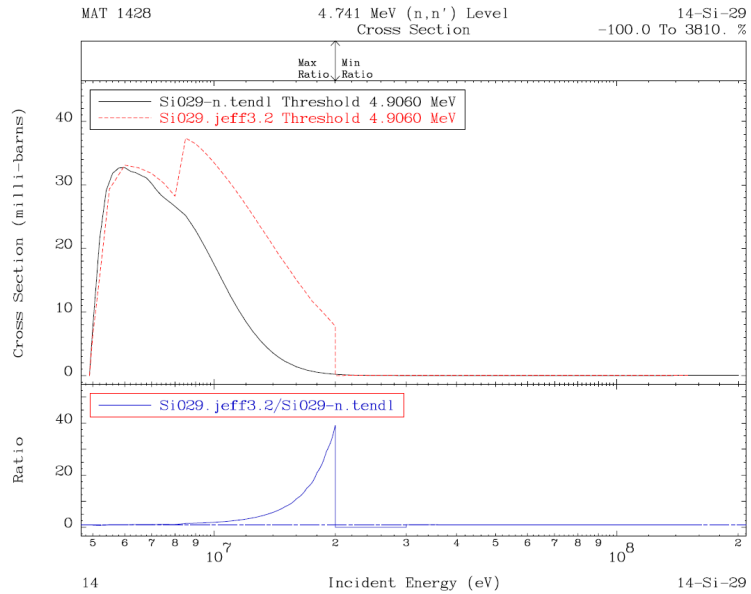


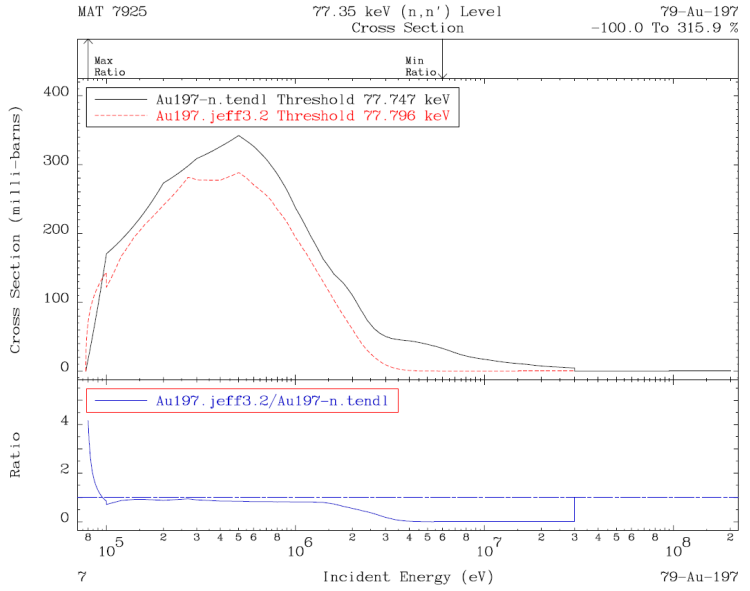


JEFF-3.2, Many specific MF3 MTs









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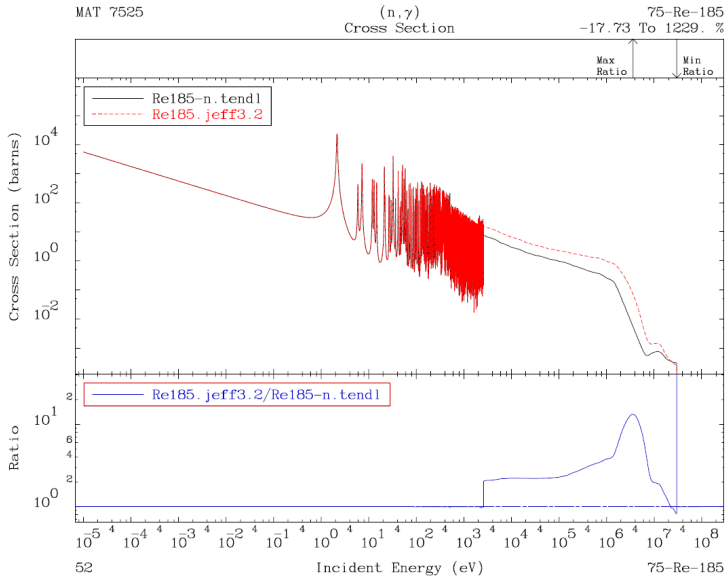
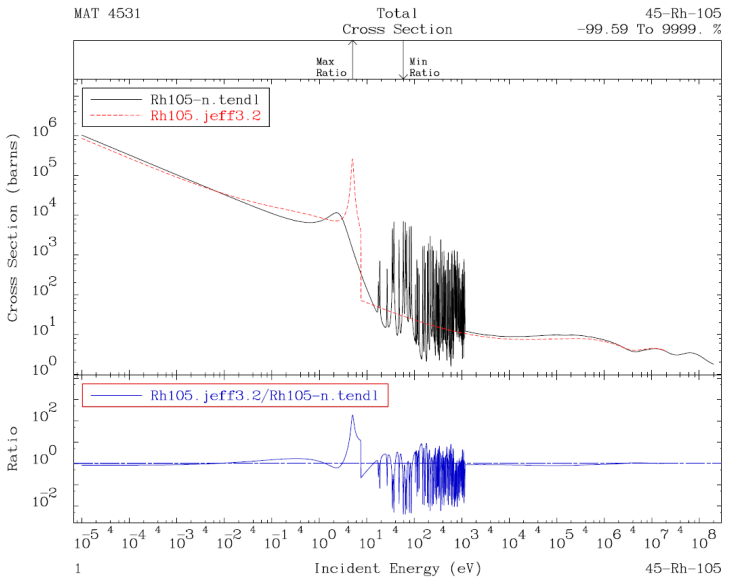
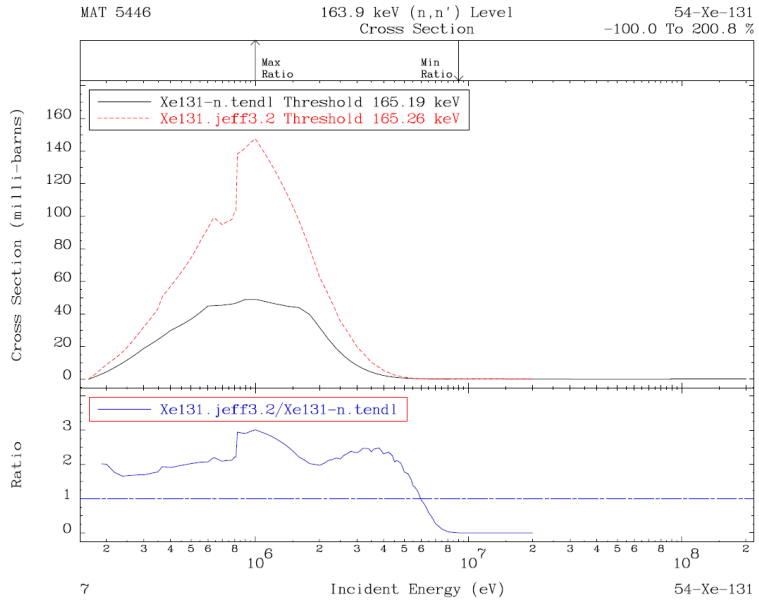
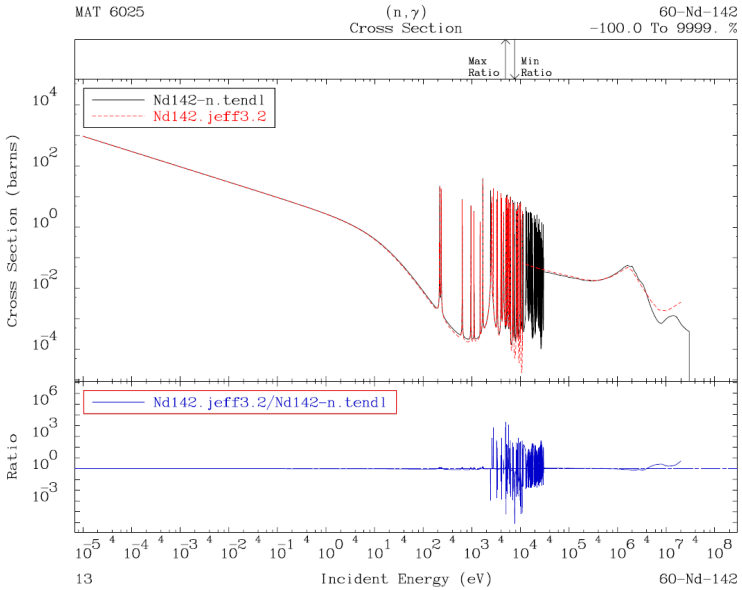








JEFF-3.2, Resonance integrals

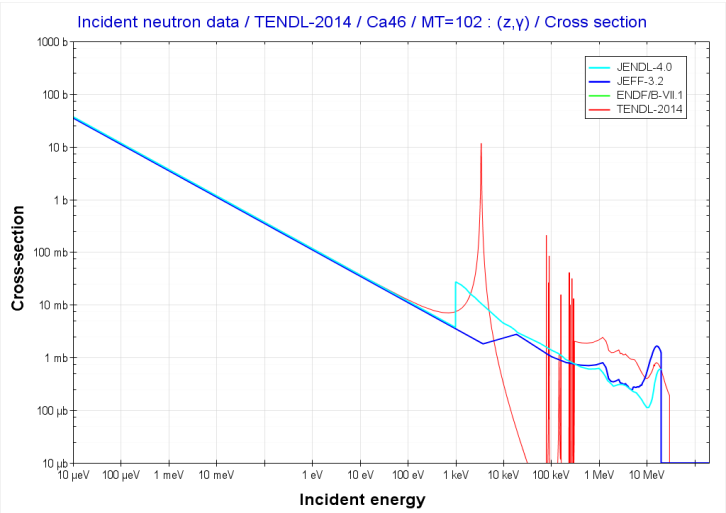
- This validation work is performed by O. Cabellos. A document is in preparation.
- Not acceptable C/E for capture/fission resonance integrals were observed for
  - ^{43}Ca, ^{46}Ca, ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, ^{50}Ti, ^{55}Mn, ^{58}Fe, ^{61}Ni, ^{62}Ni, ^{65}Cu, ^{82}Se, ^{82}Kr, ^{93}Nb, ^{96}Ru, ^{118}Sn, ^{126}Te, ^{126}Xe, ^{136}Xe, ^{135}Ba, ^{140}La, ^{142}Nd, ^{148}Nd, ^{155}Eu, ^{176}Hf, ^{178}Hf, ^{186}W, ^{204}Hg, ^{230}Th, ^{236}Pu, ^{244}Pu, ^{241}Am, ^{243}Am, ^{246}Cm, ^{250}Cf.

- Average C-E/ΔE over ≈400-600 isotopes(1) (0 means perfect agreement):

JEFF-3.2: 1.35 TENDL-2014: -0.54

JENDL-4.0: -0.37 ENDF/B-VII.1: -0.44

- Solution:
  - adjust the resonance range ?
  - change entire MF2 ?



(1) removing ^{181}Ta, ^{124}Sn, ^{236}U

JEFF-3.2: list of corrections from C. Jouanne

- This list is available in the jefdoc-1619.pdf by Cedric,
  - Negative angular distributions ^{197}Au (MF4 MT2,53, 56)
  - Negative angular distributions ^{165}Ho (MF4 MT2,51)
  - Negative angular distributions ^{239,241}U, ^{180}W (MF4 M2, 51-91)
  - Lacks in « product energy-angle distributions » ^{239}U (MF6)
  - Missing MT sections ^{168}Er, ^{189}Os
  - Missing gamma production ^{168}Er, ^{153,160}Gd, ^{189}Os, ^{27}Mg, ^{241}Pu
  - Missing gamma production

- Solution: problems corrected by C.J.

Rules for the future JEFF libraries

In the following will come propositions for a set of rules. The goal is to clarify the JEFF production and to harmonize the files.

- Simple rules for evaluations:
  - Evaluation from 0 to 200 MeV (at least) in the ENDF-6 format,
  - All-important channels included,
  - Covariance for all important reactions,
  - Documentation for the full evaluation,
  - Include in the MF1 the maximum of description, and quantities of interest (thermal, 14 MeV cross sections, MACS, resonance integrals, uncertainties...)

  - Ideally, it should all come from a production software package, no manual intervention,
  - Avoid being at the cutting-edge of the processing capabilities. We are also producing a library for users.

Rules for the future JEFF libraries

- Simple rules for processing:
  - Being processable with NJOY following a predefined set of inputs
  - Same with PREPRO, and other codes ?
  - Other processing tools like the ones developed at the NEA
  - Propose a preferred route of processing (with inputs, Oscar has done a lot of work in this field with numerous reports),
  - Provide processed files, such as tabulated cross sections and covariances, ACE, AMPX or SCALE format, pendf, gendf,... (the NEA team is already working on this),
  - For some deterministic codes, a single processed file for the complete library is necessary, shall we also produce them ?

Rules for the future JEFF libraries

- Simple rules for benchmarking:
  - Being benchmarked with relevant validations (criticality, shielding, Sinbad if possible...)
  - Use only open benchmarks, and share the input definition,
  - Use MCNP/SERPENT, other codes such as FISPACT, ?
  - Shall we pre-define a set of mandatory benchmarks ?

- Simple rules for covariances:
  - Assess the impact of the covariances on specific applications,
  - Together with covariances, random data should be provided (it makes life of users much easier)

- In case of competition with another evaluation(s), show the following:
  - Providing better benchmark results,
  - Or being more complete

Rules for the future JEFF libraries

Finally,

Just like in the case of the DICE database, it would help to have an electronic database for benchmark inputs for MCNP, Serpent, SCALE (such as Triton). This might be on voluntary basis, but many inputs are already available at many divers institutes.

- For criticality benchmarks,
- For reactor benchmarks,
- For shielding benchmarks,
- For simple systems such as used at the UAM group,
- For decay heat,
- For open-source PIE data,
- ...

Proposal for JEFF-3.3

$$\text{JEFF-3.3}^{(0)} = \text{JEFF-3.2} + \text{covariances}^{(1)} + \text{simple fixes}^{(2)}$$

Release: together with ND-2016 (Sept. 2016) and the NDS paper (Jan. 2017)

- $^{(0)}$ for all sub-libraries together
- $^{(1)}$ for all isotopes (new, or imported from other libraries)
- $^{(2)}$ as much as we can, using the lists mentioned here and possibly others

Conclusion

- We have the means to produce JEFF-3.3 with corrected evaluations,
- We have the means to produce JEFF-3.3 with covariances for all isotopes,
- We can now defined some basic rules, useful for us and the next generations (of libraries),
- Let’s do it.