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aleph

Verification and validation of a multi-temperature JEFF 3.1 library for MCNP(X)

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Introduction: Documentation is of Key Importance!

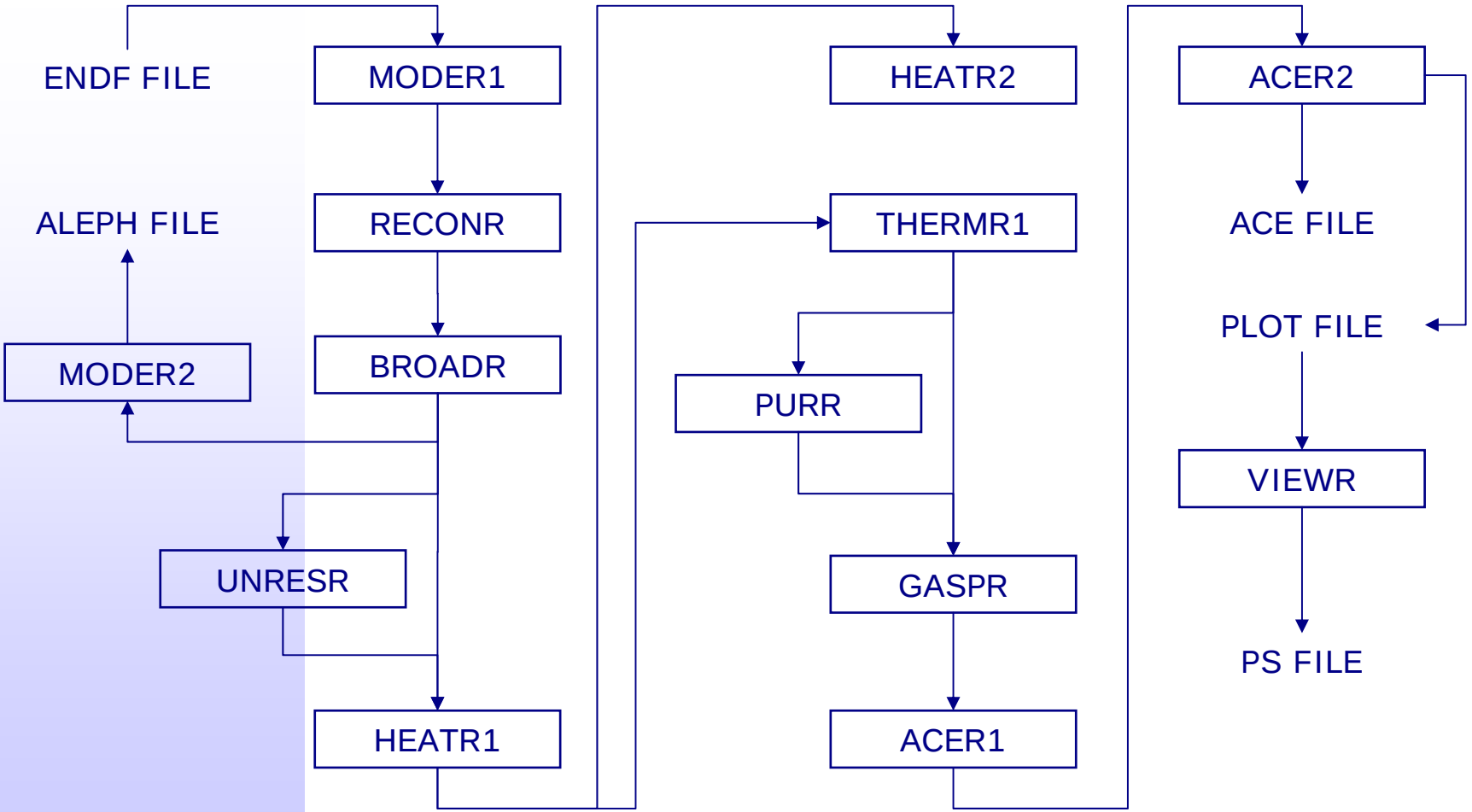
When is a set of data files to be considered a validated application library?

- When the library processing has been verified
- When the library has been tested for use
- When all aspects in its creation are thoroughly documented

Before “diving in”, it is important to know what has been done in the past:

- Look into documentation of older libraries
- The most important question in this stage: **WHY?**
- Learn from that experience and decide on your own apporach
- Good example: ENDF60 and ENDF66 from LANL
- Bad example: MCB library (no documentation at all)

Processing Path: “c” class



Automation: ALEPH-DLG

A lot of different nuclides must be processed:

- Prepare an NJOY input file tailored to every nuclide
- Check the output and perform the tests
- Tedious, repetitive and therefore error prone (“copy-paste”)

ALEPH-DLG (Data Library Generator):

- Checks important parameters (is it a fissile nuclide, does it have unresolved resonances, …)
- Makes an NJOY input file and runs NJOY
- Extracts all messages/errors and provides some comments on those messages/errors
- Performs the probability table testing

RECONR Resonance Reconstruction

The case of ^{235}U from JEFF 3.1 (default accuracy, err = 0.001)

Check the errors given and reduce the tolerance if required

Error estimates by RECONR

estimated maximum error due to resonance integral check (errmax,errint)

upper energy	elastic integral	percent error	capture integral	percent error	fission integral	percent error
1.00E-05						
1.00E-04	3.50E+01	0.000	8.15E+03	0.000	4.29E+04	0.000
1.00E-03	3.50E+01	0.000	2.57E+03	0.000	1.36E+04	0.000
1.00E-02	3.50E+01	0.000	8.02E+02	0.000	4.24E+03	0.000
1.00E-01	3.46E+01	0.000	2.15E+02	0.000	1.26E+03	0.000
1.00E+00	3.25E+01	0.000	6.03E+01	0.000	3.26E+02	0.000
...						
1.00E+02	8.30E+00	0.000	1.07E+01	0.000	2.34E+01	0.000
2.00E+02	8.04E+00	0.000	8.17E+00	0.000	1.42E+01	0.000
5.00E+02	1.10E+01	0.001	6.81E+00	0.008	1.51E+01	0.004
1.00E+03	8.28E+00	0.008	3.44E+00	0.080	7.62E+00	0.038
2.00E+03	8.27E+00	0.033	2.54E+00	0.261	5.06E+00	0.185

Something Strange

The case of elemental sulfur (S, 16000) from ENDF/B-VI.8 and ENDF/B-VII b0: the evaluation dates back to 1979.

What happened: fission widths were nonzero in the resonance parameters found in file 2.

Fixed in ENDF/B-VII b1.

RECONR resonance integral check gives non-zero fission integral?

estimated maximum error due to resonance integral check (errmax,errint)

upper energy	elastic integral	percent error	capture integral	percent error	fission integral	percent error
1.00E-05						
1.00E-04	2.26E+00	0.000	3.58E+01	0.000	1.24E-01	0.000
1.00E-03	2.26E+00	0.000	1.13E+01	0.000	3.92E-02	0.000
1.00E-02	2.26E+00	0.000	3.58E+00	0.000	1.24E-02	0.000
1.00E-01	2.26E+00	0.000	1.13E+00	0.000	3.92E-03	0.000
...						
1.00E+05	1.10E+00	0.003	1.53E-03	0.038	2.01E-03	1.743
2.00E+05	5.86E+00	0.001	2.04E-03	0.247	1.30E-03	1.077
5.00E+05	2.48E+00	0.010	1.22E-03	0.866	6.59E-04	1.765
1.00E+06	1.52E+00	0.018	5.29E-04	1.057	2.69E-05	2.025

Some Messages From NJOY

The case of non-positive elastic cross sections – RECONR:

```
---message from emerge---nonpositive elastic cross sections found.
```

Due to resonance reconstruction:

- ^{40}Ar, ^{61}Ni, ^{111}Cd, ^{113}Cd, ^{128}Te, ^{157}Gd, ^{182}W, ^{244}Cm for JEFF 3.1
- Plot it to see how “bad” it is
- Look at the other cross sections to see the overall influence

Approximations made by NJOY – HEATR:

```
---message from hinit---mf4 and 6 missing, isotropy assumed for mt 800
```

- Apparantly the corresponding file 4 (angular distribution) and/or file 6 (energy-angle distributions) are missing. HEATR has to make an assumption for the missing data.

ACER Consistency Tests

The case of ^{11}B from JEFF 3.1

No problems found!

```
ace consistency checks
----------------------
check reaction thresholds against q values
check that main energy grid is monotonic
check angular distributions for correct reference frame
check angular distributions for unreasonable cosine values
check energy distributions
check photon production sum
check photon distributions
checking particle production sections
  proton production:
  checking energy distributions
  alpha production:
  checking energy distributions
no problems found
```

Further Post-Processing and Testing

If we look at ENDF60 and ENDF66, the following post-processing and testing was performed:

- Add other data like delayed neutrons, gas production data, ... (which is now done by ACER, GASPR, ...)
- CHECKTHRESH: check the threshold energy versus the Q-value (now performed and corrected by RECONR and ACER)
- CHECKNS and CHECKND_NEUT: check the photon and delayed neutron distributions (now performed by ACER)
- CHECK5: check data files with the mt5 reaction
- CHECK_URES: check the probability tables for consistency

Only the probability tables are not (yet) extensively tested by NJOY.

Probability Table Testing (1)

Compare the infinite dilution cross sections from UNRESR and PURR

The case of ^{238}U of JEFF 3.1 (E = 20 keV) :

	total	elastic	fission	capture	unresr tot	purr tot
unresr	1.432516E+01	1.379577E+01	0.000000E+00	5.293905E-01	1.432516E+01	1.432516E+01
purr infd	1.432516E+01	1.379577E+01	0.000000E+00	5.293905E-01		
purr bkgd	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00		
diff [%]	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
passed?	yes	yes	yes	yes	yes	yes

The case of ^{241}Pu of JEFF 3.1 (E = 30 keV) :

	total	elastic	fission	capture	unresr tot	purr tot
unresr	1.411443E+01	1.084413E+01	2.603048E+00	5.307552E-01	1.397793E+01	1.411443E+01
purr infd	1.411443E+01	1.084413E+01	2.739547E+00	5.307552E-01		
purr bkgd	1.673491E-01	0.000000E+00	1.364989E-01	3.085028E-02		
diff [%]	0.0000	0.0000	5.1098	0.0000	0.9718	0.0000
passed?	yes	yes	no	yes	no	yes

What if the unresr-purr test fails?

Probability Table Testing (2)

Compare Bondarenko table from direct sampling and the probability table

The case of ^{238}U of JEFF 3.1 (E = 20 keV) :

Bondarenko cross sections by direct sampling

sigma0	p0 total	elastic	fission	capture	p1 total
1.000000E+10	1.436541E+01	1.383465E+01	0.000000E+00	5.307606E-01	1.436541E+01
...					
1.000000E+01	1.316814E+01	1.268519E+01	0.000000E+00	4.829514E-01	1.234338E+01

Bondarenko cross sections from probability table

sigma0	p0 total	elastic	fission	capture	p1 total
1.000000E+10	1.436541E+01	1.383465E+01	0.000000E+00	5.307606E-01	1.436541E+01
...					
1.000000E+01	1.318591E+01	1.270308E+01	0.000000E+00	4.828283E-01	1.236715E+01

Bondarenko cross sections difference [%]

sigma0	p0 total	elastic	fission	capture	p1 total
1.000000E+10	0.0000	0.0000	0.0000	0.0000	0.0000
...					
1.000000E+01	0.1349	0.1409	0.0000	0.0255	0.1924

Probability Table Testing (3)

Check the probability table for consistency:

- Does the sum of the partials equal the total in every bin?
- Does the average from the probability table equal that of the ladder calculation?
- Are there no abnormalities (zeros or negatives)?

The case of ^{238}U of JEFF 3.1 (E = 20 keV) :

bin	tot prob	cum prob	total	elastic	fission	capture
1	4.662500E-03	4.662500E-03	3.823343E+00	3.585895E+00	0.000000E+00	2.374473E-01
2	1.791875E-02	2.258125E-02	6.229751E+00	5.966992E+00	0.000000E+00	2.627585E-01
3	6.367188E-02	8.625313E-02	8.460657E+00	8.200861E+00	0.000000E+00	2.597957E-01
...						
18	6.582813E-02	9.753844E-01	2.653817E+01	2.553805E+01	0.000000E+00	1.000119E+00
19	1.940000E-02	9.947844E-01	4.153256E+01	4.053079E+01	0.000000E+00	1.001761E+00
20	5.215625E-03	1.000000E+00	5.675590E+01	5.566543E+01	0.000000E+00	1.090471E+00
	average probability table		1.436541E+01	1.383465E+01	0.000000E+00	5.307606E-01
	average ladder calculation		1.436541E+01	1.383465E+01	0.000000E+00	5.307606E-01
		diff [%]	0.0000	0.0000	0.0000	0.0000
		passed?	yes	yes	yes	yes

Probability Table Testing (4)

The case of ^{22}Na of JEFF 3.1 (E = 15 keV) :

bin	tot prob	cum prob	total	elastic	fission	capture
1	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
...						
9	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
10	5.852375E-01	5.852375E-01	1.056769E-01	0.000000E+00	0.000000E+00	-3.959991E-02
...						
12	3.425000E-02	6.523844E-01	1.056858E-01	0.000000E+00	0.000000E+00	-3.959101E-02
13	6.732500E-02	7.197094E-01	1.057690E-01	1.138332E-08	0.000000E+00	-3.950781E-02
...						
17	5.180000E-02	9.476781E-01	2.888497E+00	2.760378E+00	0.000000E+00	-1.715786E-02
18	3.734063E-02	9.850187E-01	1.538414E+01	1.514680E+01	0.000000E+00	9.206328E-02
...						
20	4.143750E-03	1.000000E-00	9.958044E+01	9.904143E+01	0.000000E+00	3.937373E-01
	average probability table		1.912509E+00	1.793225E+00	0.000000E+00	-2.599318E-02
	average ladder calculation		1.912509E+00	1.793225E+00	0.000000E+00	-2.599318E-02
		diff [%]	0.0000	0.0000	0.0000	0.0000
		passed?	yes	yes	yes	yes

Zero probability bins

Zero cross section values

Negative cross section values

Library Validation (1)

Now that the libraries are ready, we can test them against internationally accepted benchmarks.

It is impossible to benchmark everything so choices must be made:

- Criticality benchmarks:

  Taken from LA-13594 – these were prepared for the purpose of validating nuclear data

  Covers a wide range of materials

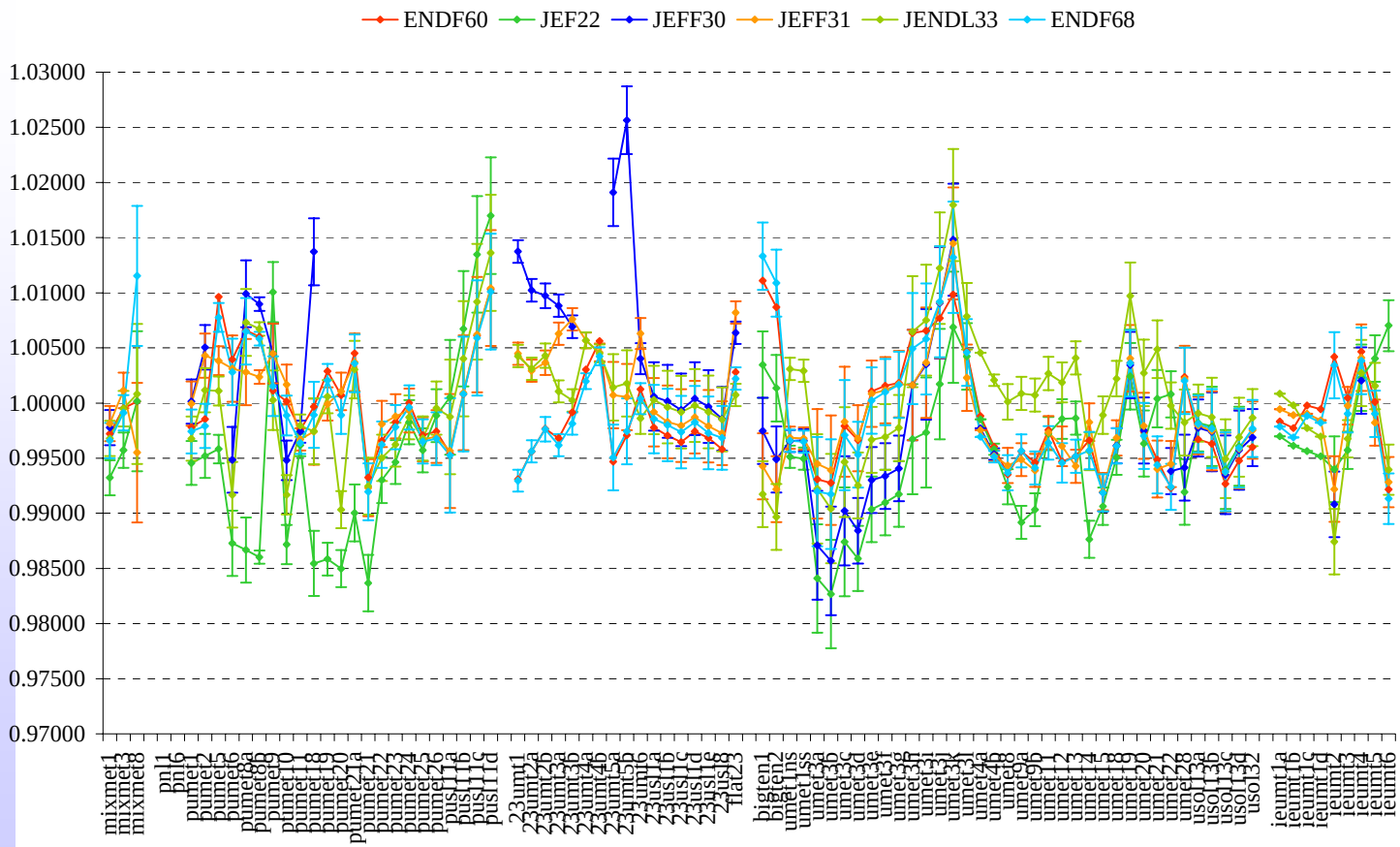
- Lawrence Livermore Pulsed Sphere Experiments:

  Time of flight – tests data between 2-16 MeV

  Often single material experiments

Library Validation (2)

C/E results for the criticality benchmarks.

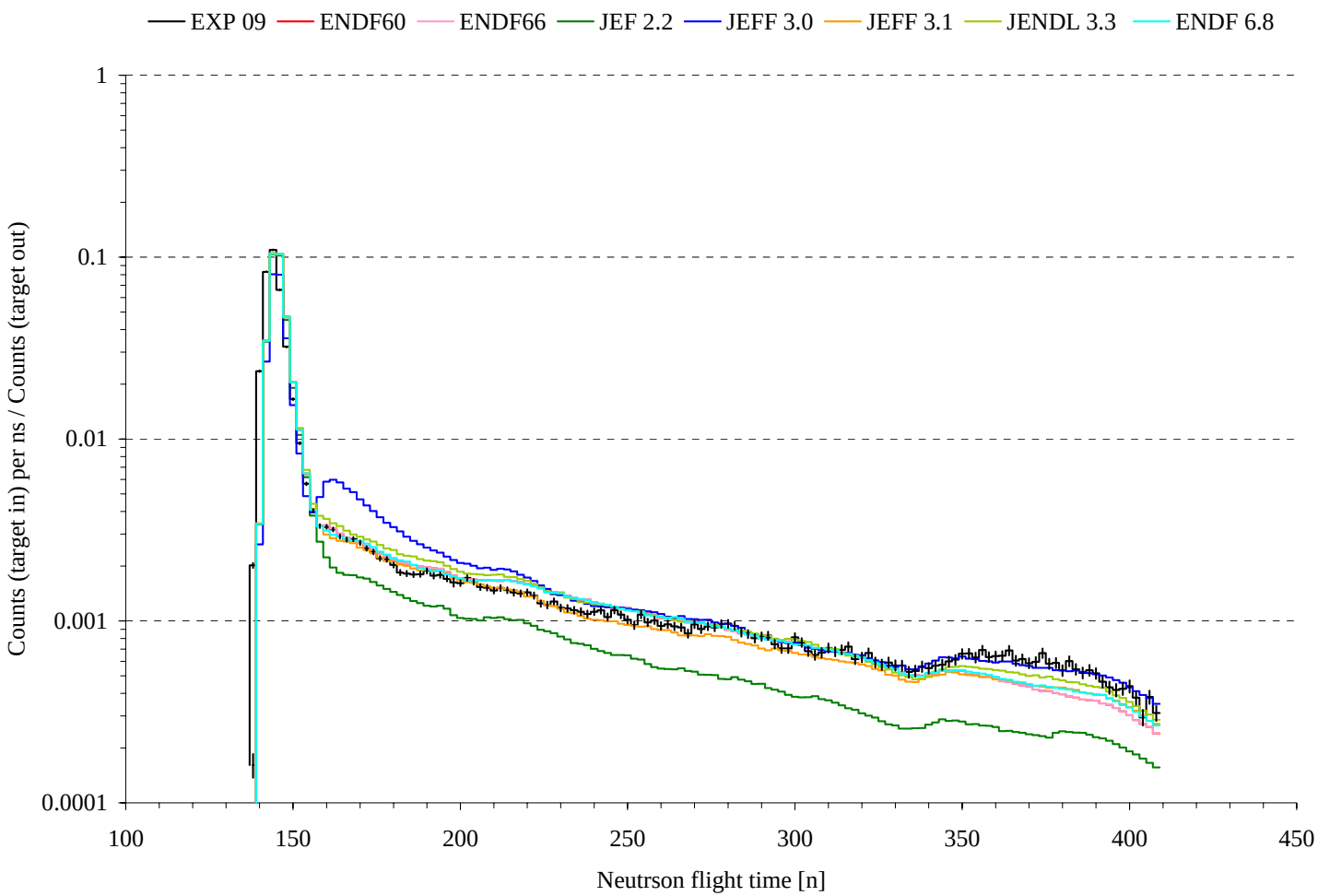


Library Validation (3)

Time of flight results for a beryllium sphere.

30 degrees

765.2 cm

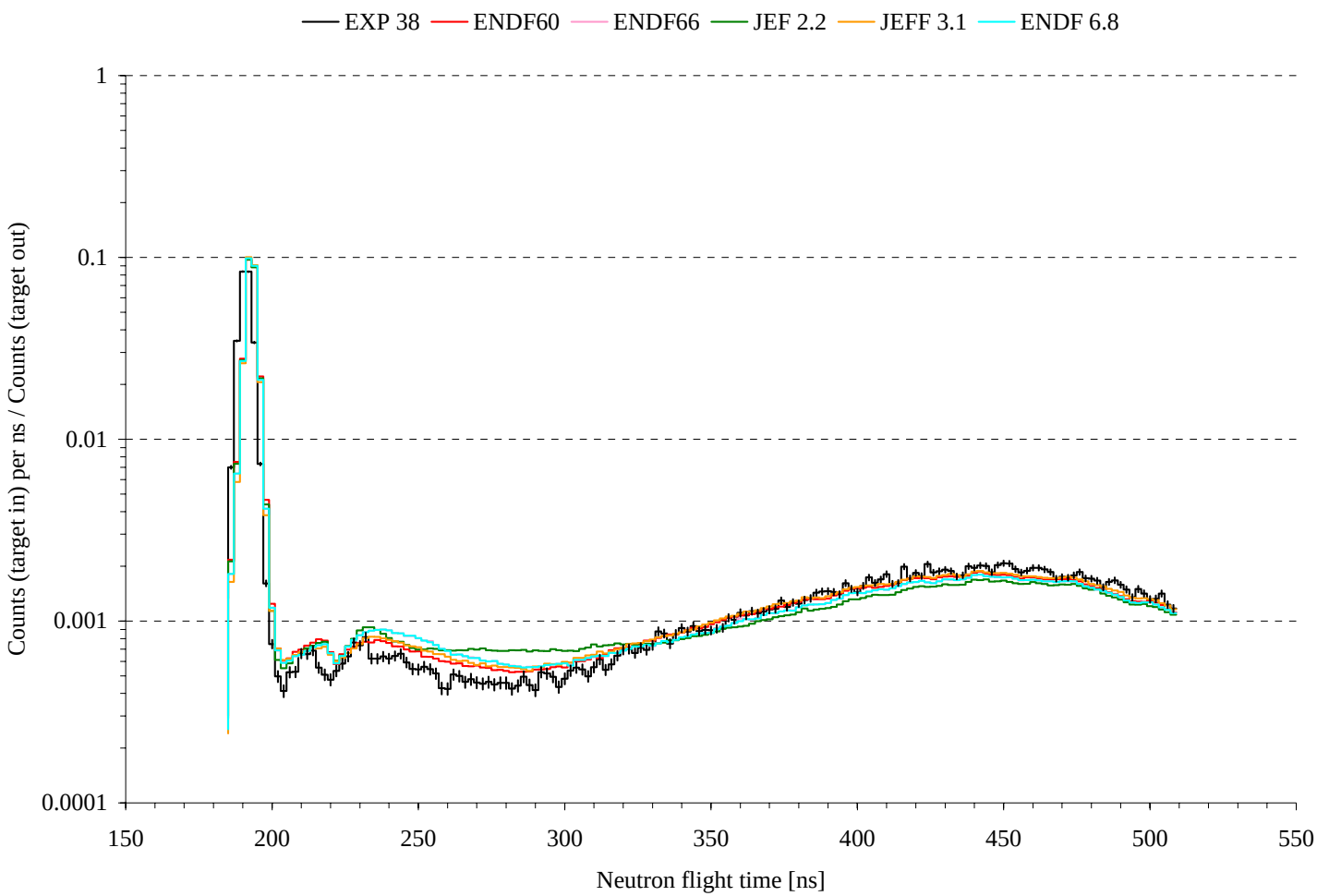


Library Validation (4)

Time of flight results for a lead sphere.

120 degrees

975.2 cm



Conclusions

The presented approach assures quality:

- Automation in ALEPH-DLG avoids “copy-paste” errors
- Important NJOY output is extracted and reviewed
- Testing is performed where NJOY lacks testing
- Extensive documentation
- However: there is still room for improvement, and that is where the nuclear data community comes in

ALEPH-LIB is currently:

- Neutron data at 300, 600, 900, 1200, 1500 and 1800 K
- JEF 2.2, JEFF 3.0, JEFF 3.1, JENDL 3.3 and ENDF/B-VI.8

Future additions:

- ENDF/B-VII
- S(α,β) data
- Proton data

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Any Questions?

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