Updating the NJOY2016.72 code for processing FENDL

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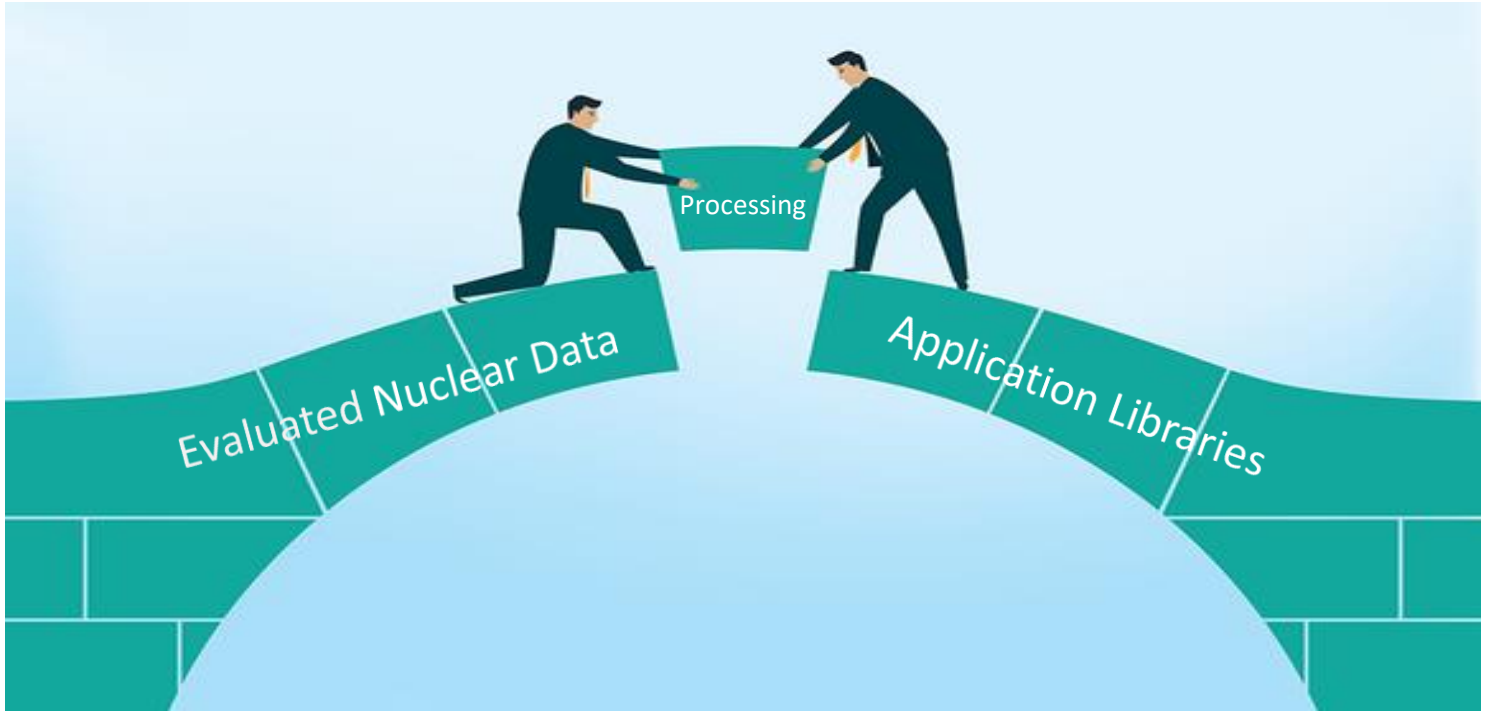
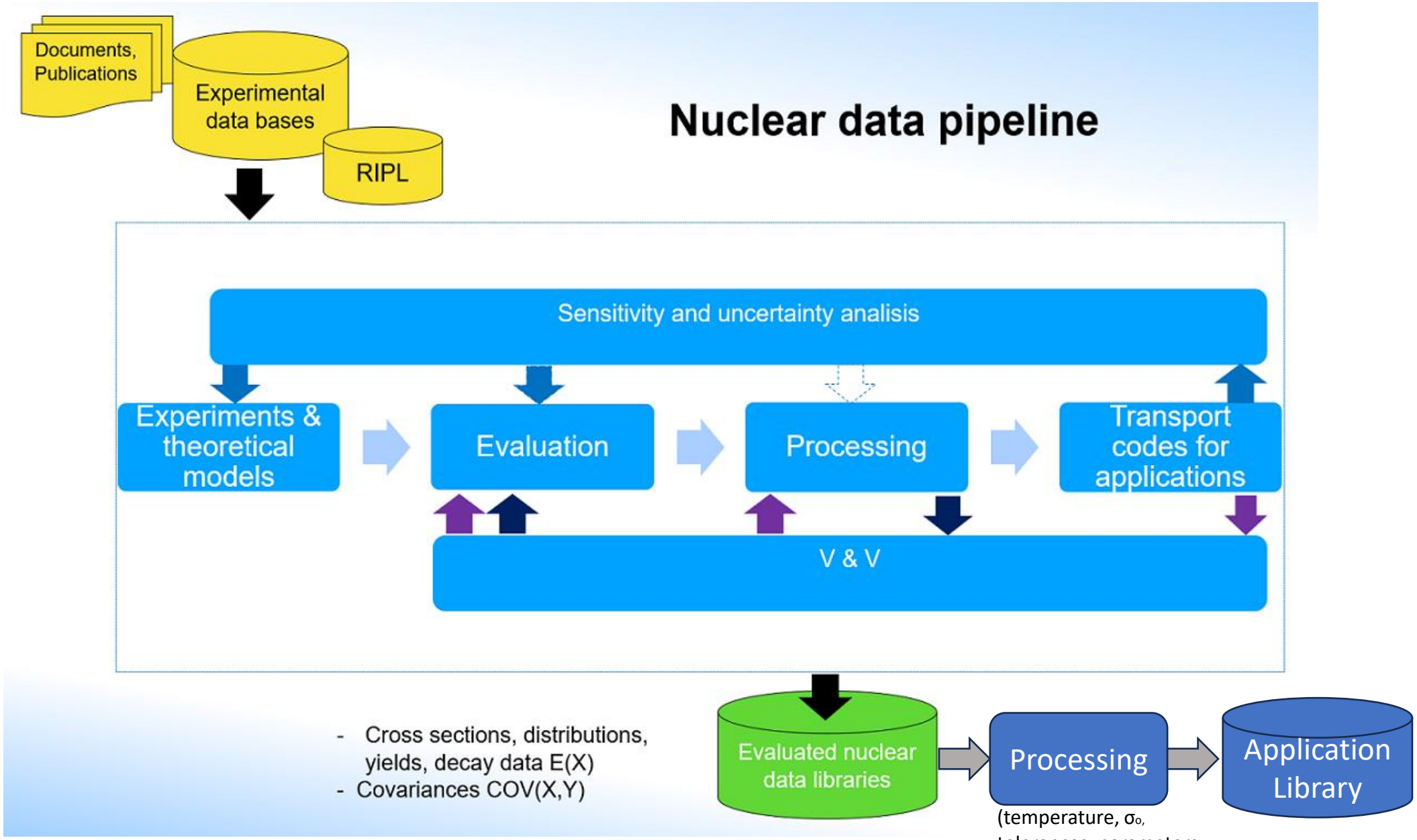
Outline

1. Introduction
2. Main updates for processing FENDL using NJOY2016.72
3. Final comments

1. Introduction



Nuclear data pipeline



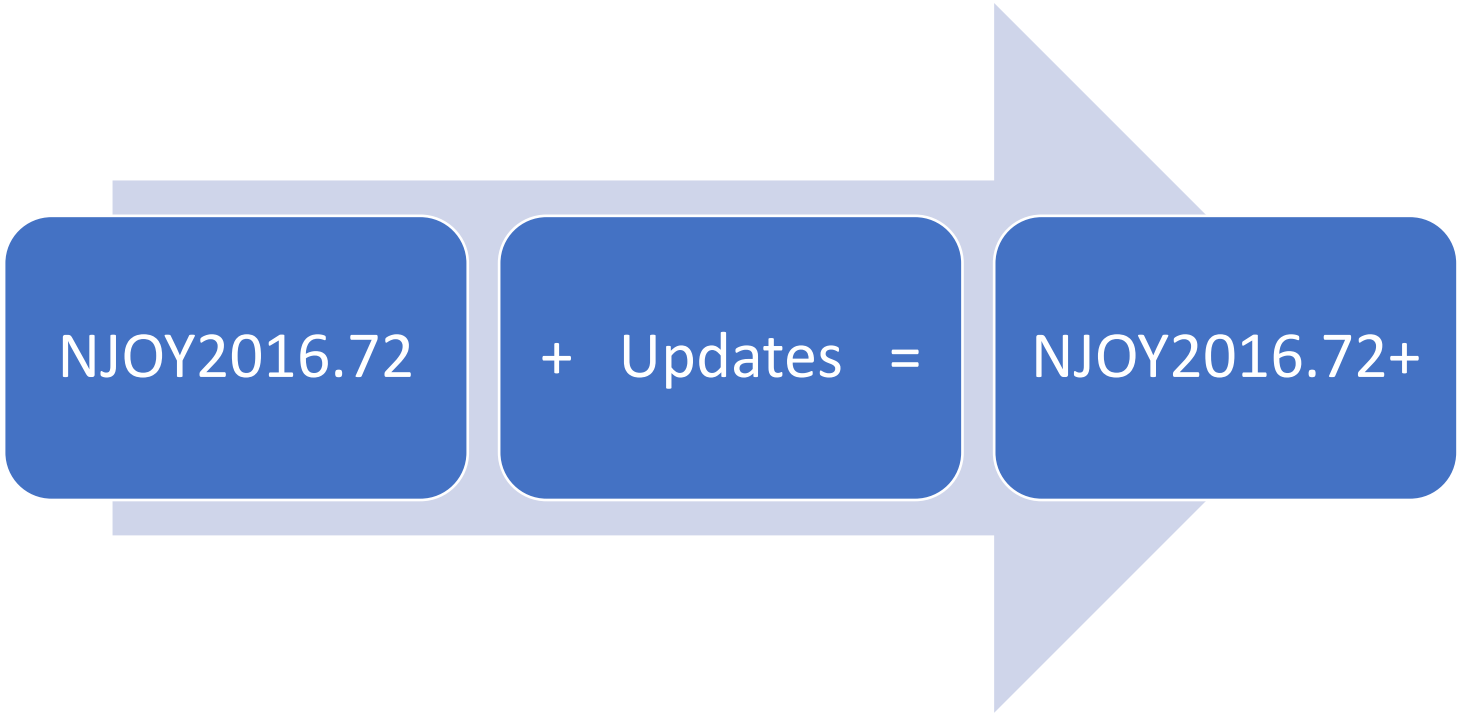
- The FENDL application libraries were prepared using different versions of the NJOY processing system
- Processing is required after any correction or improvement of the evaluated data or any correction or improvement of the processing methods
- Local patches were always needed taking into account the feedbacks from the verification and validation procedures (V&V)
- Suggestions from users and library testers have been continuously incorporated
- FENDL application libraries are available on https://www-nds.iaea.org/fendl/

Library version	NJOY versions used for processing	Year
FENDL-2.1 (ITER design)	NJOY-99.90 + updates	2004
FENDL-3.0	NJOY-99.364 + updates	2011
FENDL-3.1,-3.1a, b, c, d	NJOY-2012.50 … .145 + updates	2015,2016,2017,2018
FENDL-3.2,-3.2a, b	NJOY-2016.60 … .67 + updates	2021,2022

- The updates were systematically adapted/traslated between NJOY versions
- Kind of updates for FENDL
  a) Including new features or extending the coded ones
  b) Correcting bugs in coding and adding extra checking
  c) Increasing arrays size
  d) Implementation for different compilers (gfortran & lahey)
  e) Updating version numbers and comments
- Some updates proposed in the frame of FENDL project have been completely or partially included in the official releases of the NJOY code, but not all
- Still some updates are required for processing FENDL
- The updated version of the NJOY2016 code for processing FENDL is available on https://github.com/IAEA-NDS/NJOY2016

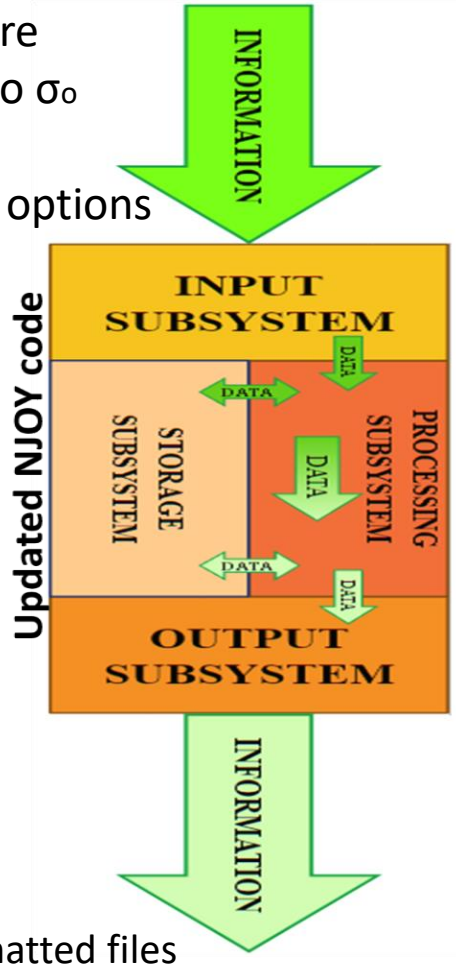
- Recently, the codes NJOY2016.71 and NJOY2016.72 (released on September 28) were updated to be ready for generating the FENDL applications libraries (Currently FENDL-3.2b)
- The updates are essentially the same for version .71 and .72, but in version .72 one of the proposed updates was considered by the NJOY developers at LANL
- It is worthy to note, that most of the updates proposed for processing FENDL are also required for processing other evaluated nuclear data libraries like the ENDF/B-VIII.0, JENDL-5 and TENDL-2021
- There are updates for incident neutrons and charged particles
- All the updates were sent to the NJOY developers at LANL for checking
- Additionally, updates required for generating other applications libraries distributed by the NDS/IAEA like the IRDFF-II, ADS-2.0, WIMSD are also included
- Updated modules (24/39): acecm, acedo, acefc, acepa, acepn, acer, broadr, endf, errorr, gaspr, groupr, heatr, leapr, locale, main, mainio, matxsr, plotr, purr, reconr, util, vers, viewr, wimsr

2. Main updates for processing FENDL using NJOY2016.72



FENDL (ENDF-format)

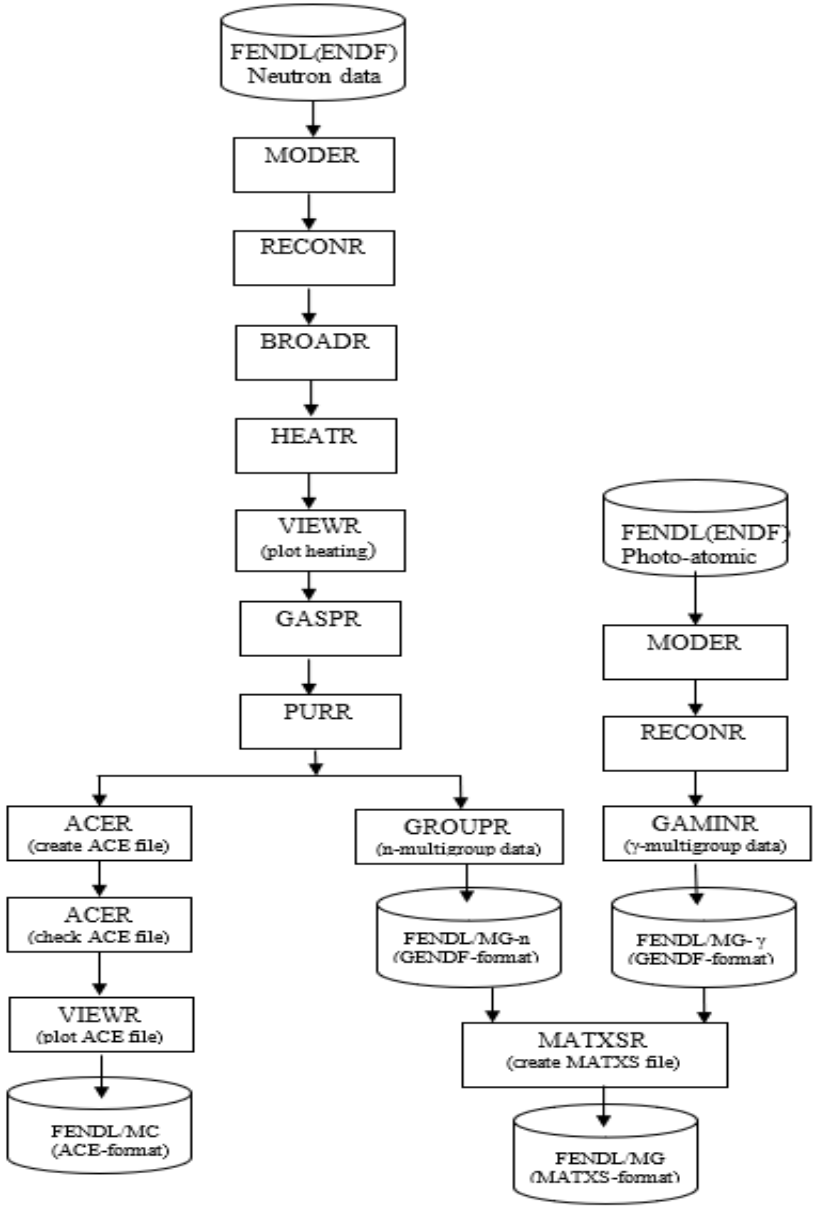
Temperature
Bondarenko σ_0
Tolerances
Processing options



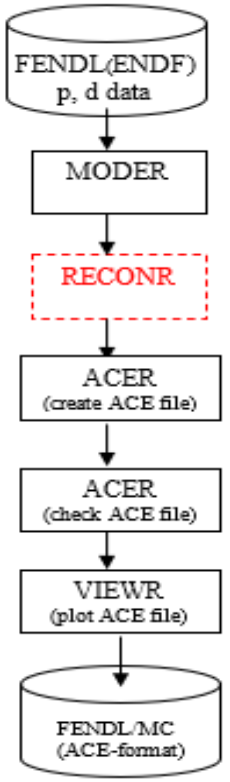
Output formatted files
- ACE
- MATXS
- GENDF

FENDL Application libraries

Incident neutrons



Incident charged particles (protons, deuterons)



NJOY module	FORTRAN module	Comments on more important updates
reconr	reconr.f90	1. Implemented the possibility of use reconr for linearizing charged particle evaluations. 2. Implemented the correct treatment of the elastic scattering cross section for charged particles. For mf6/law5/ltp≥12, the mf3/mt2 section should contain the values of the "nuclear plus interference" cross section σ_{NI}, which can be negative. For ltp=1 or ltp=2, the values should be 1.0 even at the threshold energy. Otherwise, the elastic scattering cross section could be incorrectly calculated in *subroutine acecpe*. 3. Built-up of redundant reactions removed for charged particles
broadr	broadr.f90	1. Minor just to be compatible with LAHEY FORTRAN

NJOY module	FORTRAN module	Comments on more important updates
heatr	heatr.f90	• Heating number = the upper kinematic limit (Mr. Chikara Konno, Mr. Kazuaki Kosako) • Correction of the recoil energy calculation for reaction MT=102(n, g) [Wen Yin et. al. (2021)]
gaspr	gaspr.f90	• Li-8 -> beta decay -> Be-8 -> 2 alpha particles. (Important for light nuclides like Boron)
purr	purr.f90	• Implemented a procedure for managing very small total cross section during sampling. It was important for processing La-139 from FENDL-3.1 [1] Chikara Konno, Kenichi Tada, Saerom Kwon, "MATXS multigroup file problem due to NJOY unresolved resonance processing", ICRS14/RPSD2020, 2020 [2] Lopez Aldama, D., Capote Noy, R., "Processing La-139 in the Unresolved Resonance Region for the FENDL Library", INDC(NDS)-0825, International Nuclear Data Committee, IAEA

NJOY module	FORTRAN module	Comments on more important updates
acer	acecm.f90 acer.f90 acefc.f90	1. Starting from the Japanese updates for processing incident charged particle from JENDL-5 a new input option was implemented for controlling whether the endf/mf6/law7 is converted to ace/law61 or to ace/law61 when the new format option (newfor=1) is invoked. [Modification of NJOY2016.65 for JENDL-5 neutron, photo-atomic, and charged particle sub-libraries, at JENDL-5 web page] 1. Added checking and plotting capabilities of law67 2. Correction of ZA and AWR values for charged particles in several subroutines (neutron data was used) 3. Patching the inclusion of extra-points in the unified energy grid for large energy subintervals in the case of charged particles

NJOY module	FORTRAN module	Comments on more important updates
acer	acecm.f90 acer.f90 acefc.f90	5. Patching the case when only MT2 produce the incident particle (NJOY2016.72 crashed) 6. Warning when LAB reference system is used for endf/mf6/law6. CM system is expected and NJOY2016 assumes (1-H-2 from JENDL-5 proton library) 7. Correction to the smoothing option of NJOY2016 for histograms when the first secondary energy is not 0.0 or less than 1.0E-5 eV using Kalbach-Mann representation. (problem for some TENDL files) 8. Correction to avoid singularities at μ=1.0 when the scattering cross section for charged particles is calculated (NJOY2016.72 crashed)

NJOY module	FORTRAN module	Comments on more important updates
acer	acecm.f90 acer.f90 acefc.f90	9. Revisiting the logic for include producing- and non-producing incident particles 10. Minor coding reordering and increasing of several arrays size
groupr	groupr.f90	1. Minor code reordering and increasing the size of some arrays.
matxsr	matxsr.f90	1. A FORTRAN format descriptor was corrected. It produces wrong data when matxs-formatted (ASCII) files are generated.

NJOY module	FORTRAN module	Comments on more important updates
viewr	viewr.f90	1. Increase some arrays dimension for large plots
endf	endf.f90	1. Rewind the tape before using it in subroutine tpidio. Needed when running multiple modules in sequence.
util	util.f90	1. Close the scratch tape before opening it in *subroutine openz*, if needed *2. Minor correction in function sigfig*

- HEATR new update is the only one that directly affects neutron data
- Wen Yin, Tiejun Zu, Liangzhi Cao, Hongchun Wu, “Remarks and improvements on neutron KERMA factors and radiation damage cross sections calculated by NECP-Atlas and NJOY21 using different evaluated nuclear data libraries”, Annals of Nuclear Energy 164 (2021) 108624
- The issue is related to the recoil energy of MT102 (n,g) in NJOY:

If MF4/MF5 data available:

$$E_R = \frac{E}{A+1} + \frac{Y\,(\bar{E_\gamma})^2}{2(A+1)mc^2}$$

If MF6 data available:

$$E_R = \frac{E}{A+1} + \frac{(\bar{E_\gamma})^2}{2(A+1)mc^2};$$

The correct expression:

$$E_R(E) = \frac{E}{A+1} + \frac{(YE_\gamma)^2}{2(A+1)mc^2}$$

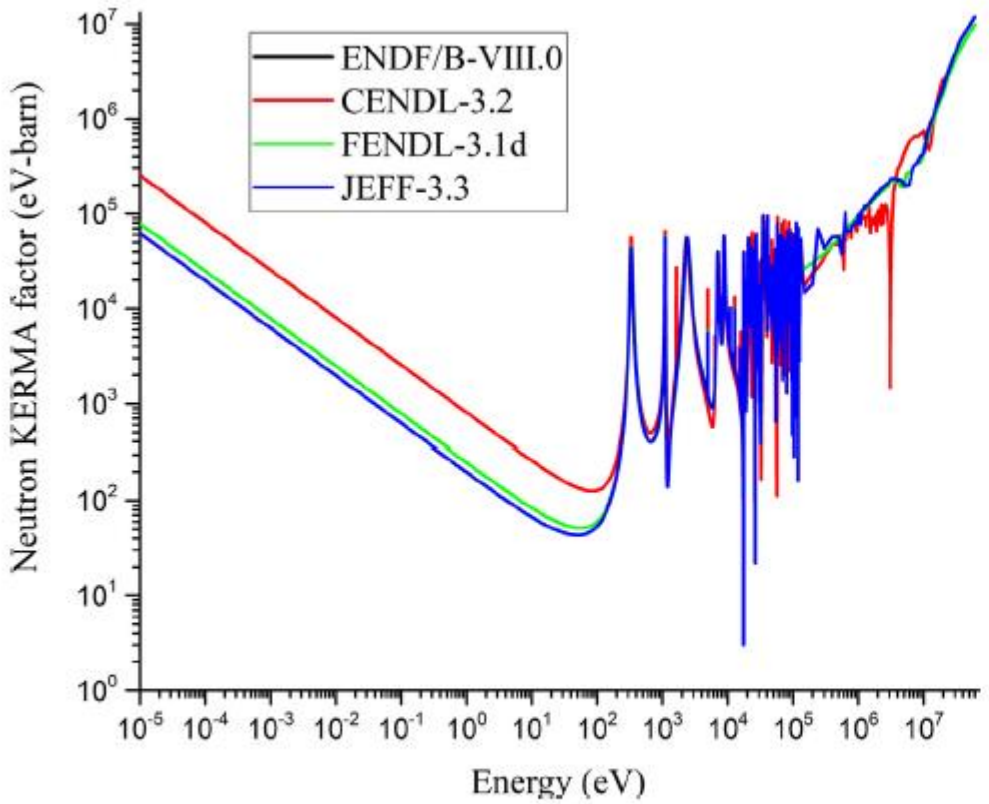


Fig. 1. KERMA factors of ^{55}Mn calculated by NJOY21 based on different ENDFs.

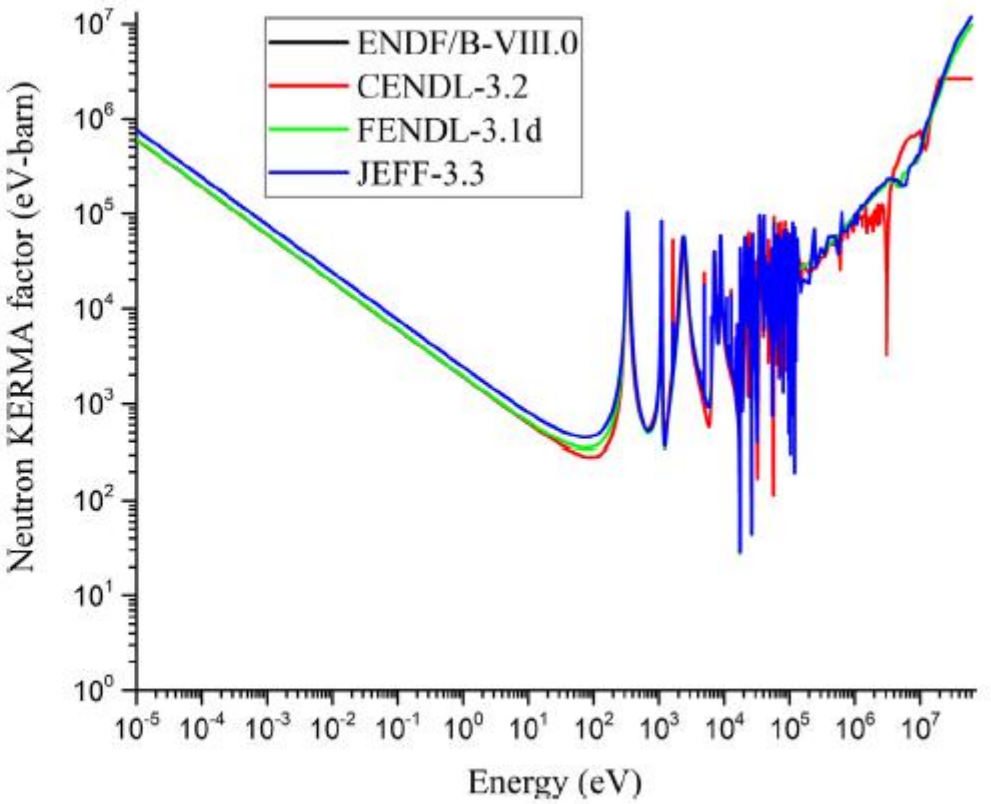
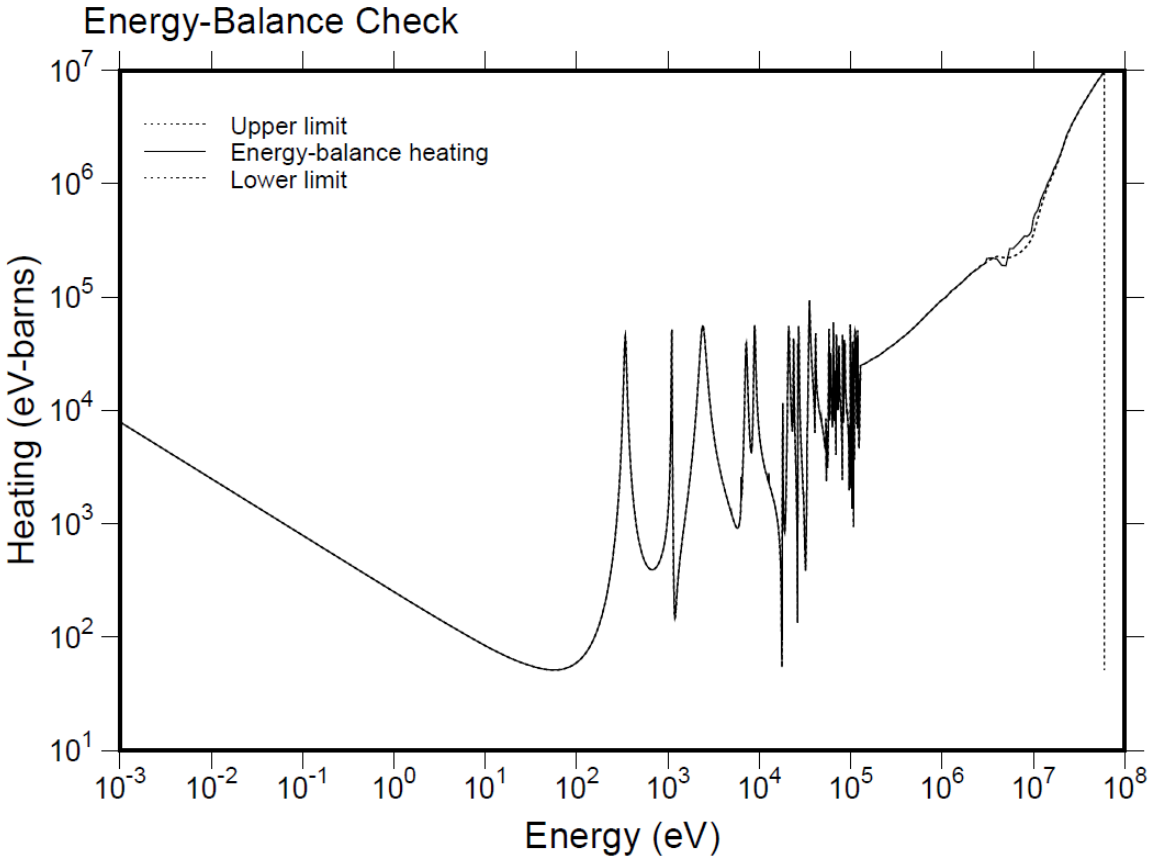


Fig. 3. KERMA factors of ^{55}Mn calculated by NECP-Atlas based on different ENDFs.

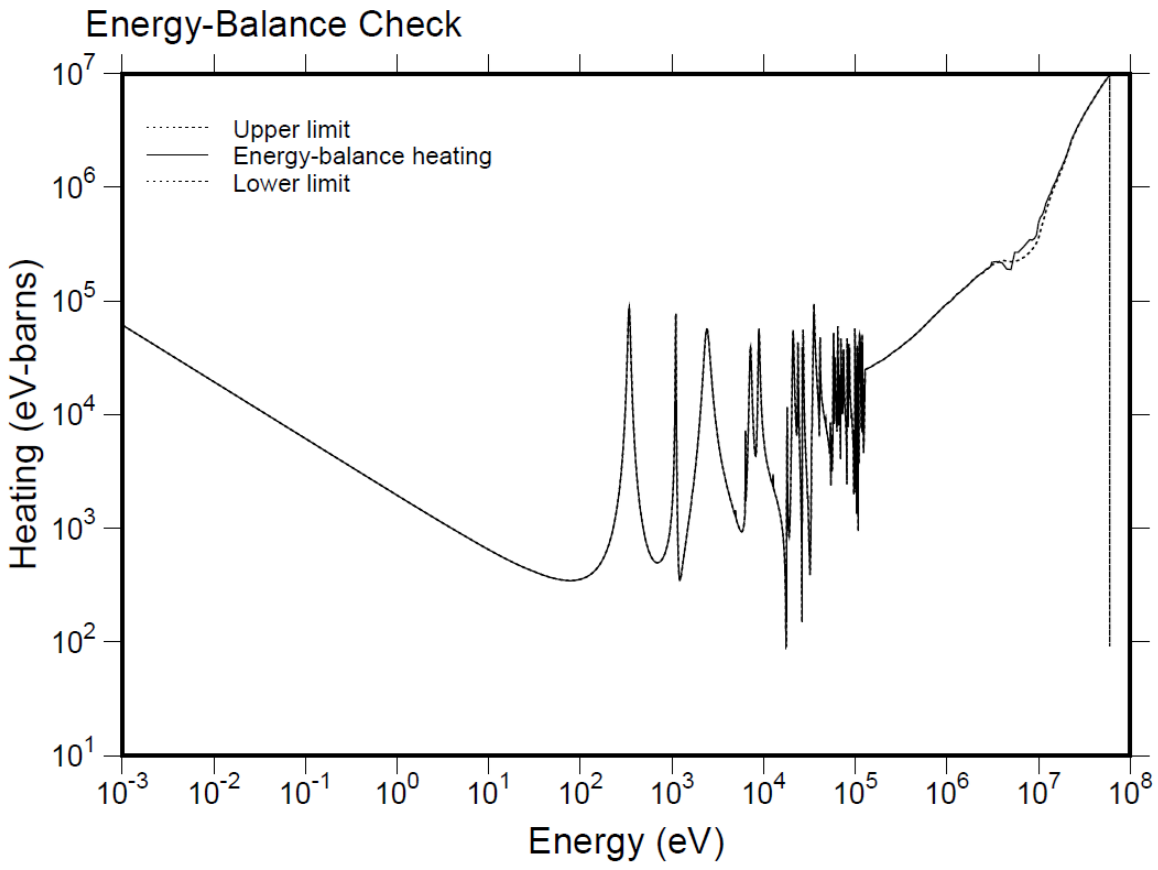
Source: Wen Yin et. al. (2021)

Mn-55 from FENDL-3.2b (INDL/V-3 evaluation)

Without the update



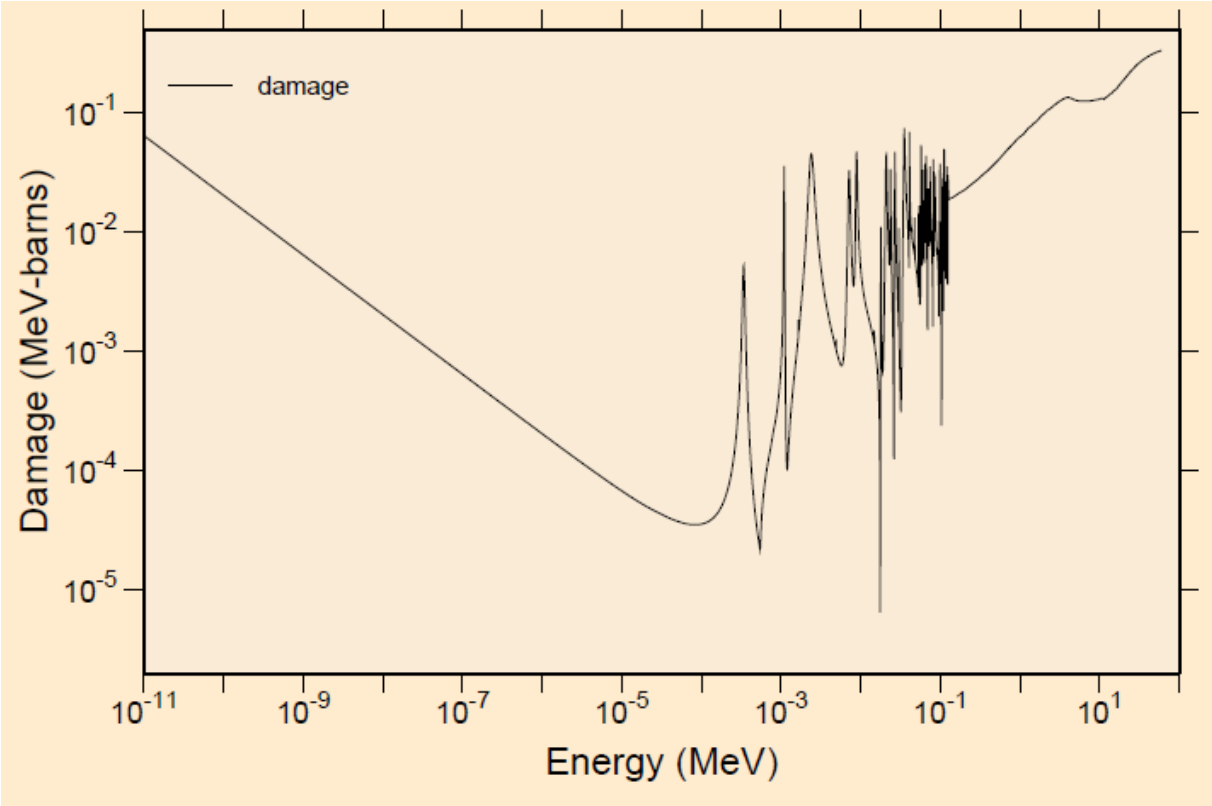
Updated



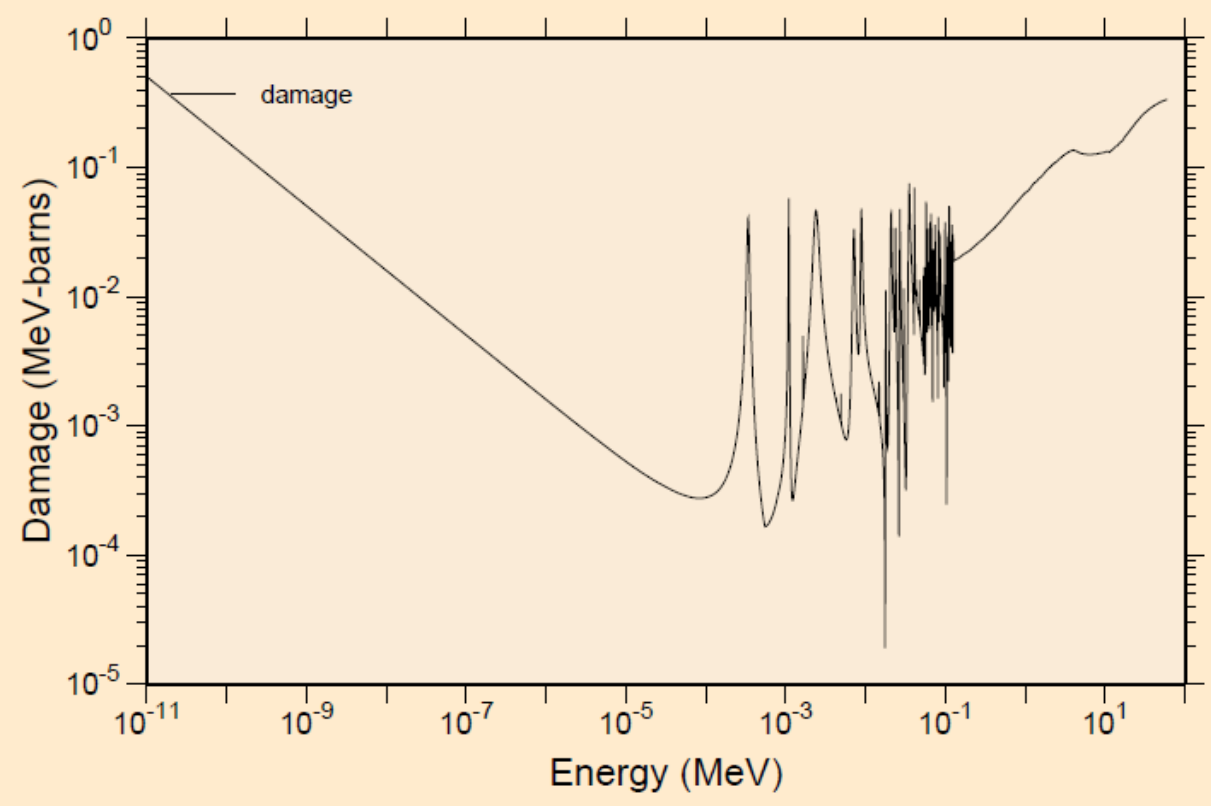
1 order of magnitude at low energies!!!

Mn-55 from FENDL-3.2b (INDL/V-3 evaluation)

Without the update

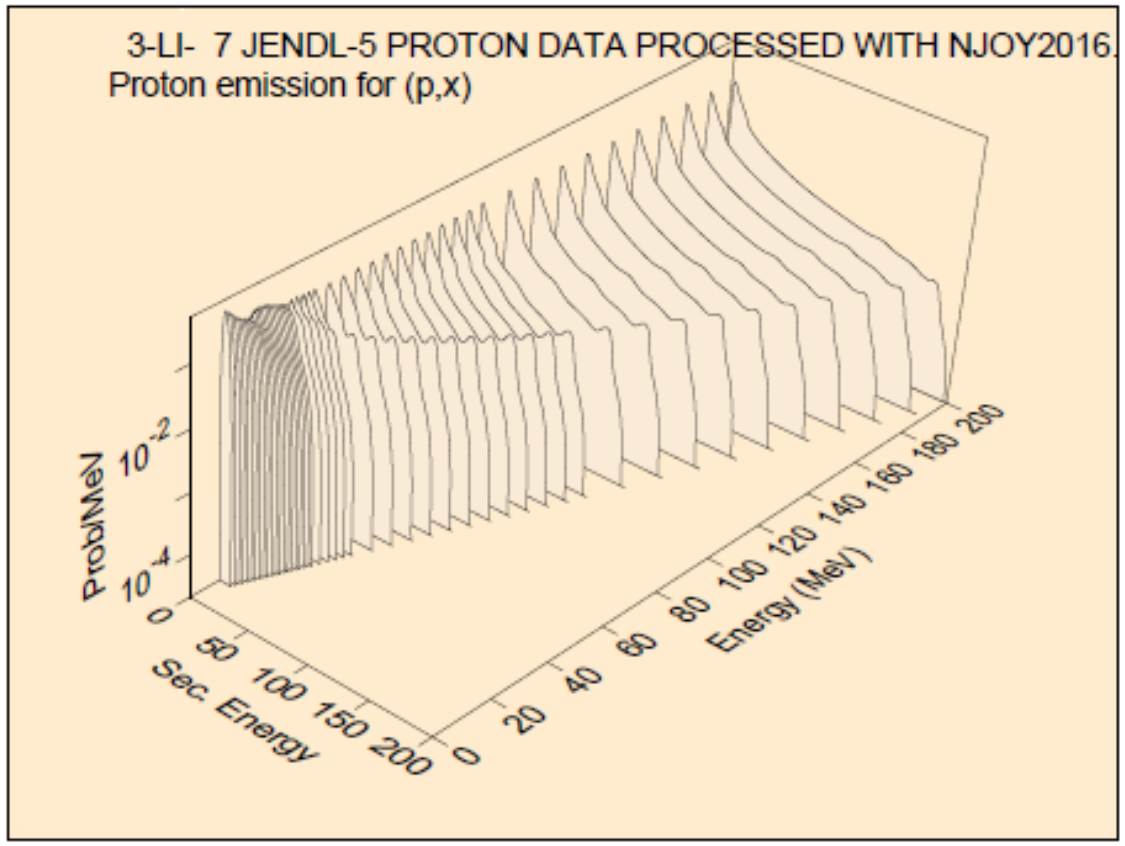


Updated

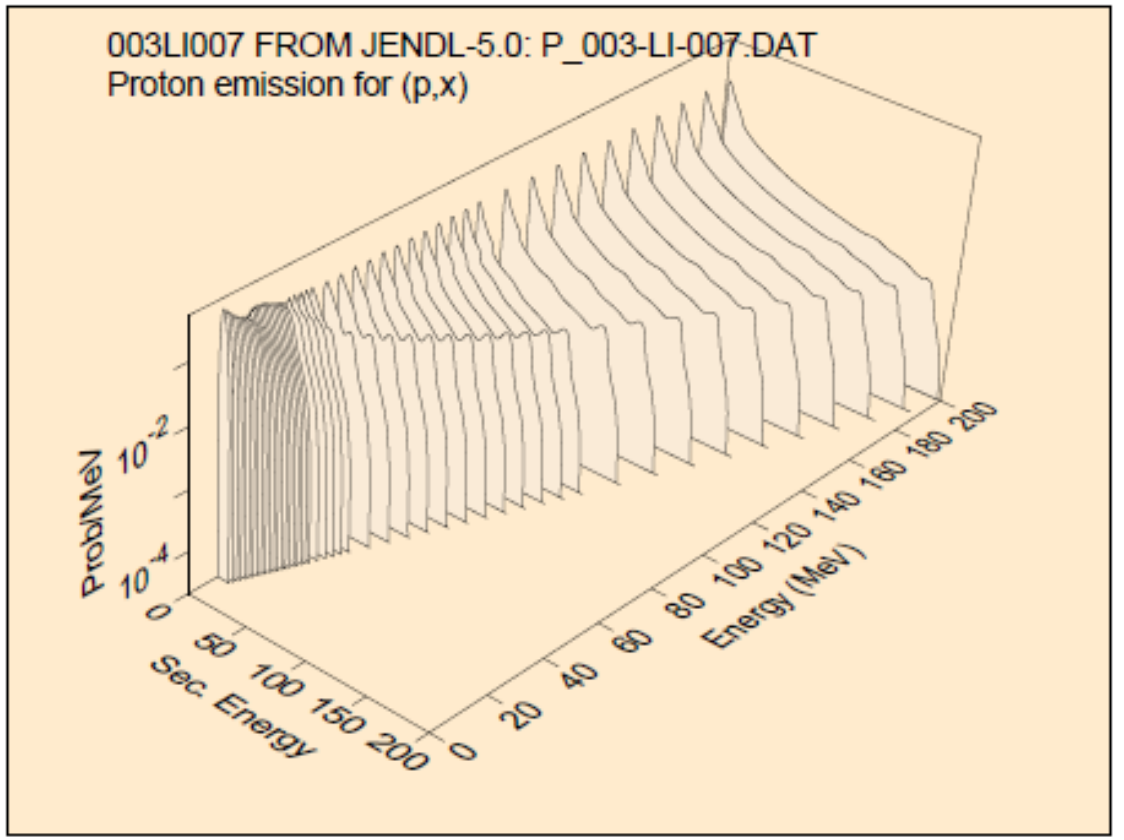


1 order of magnitude at low energies!!!

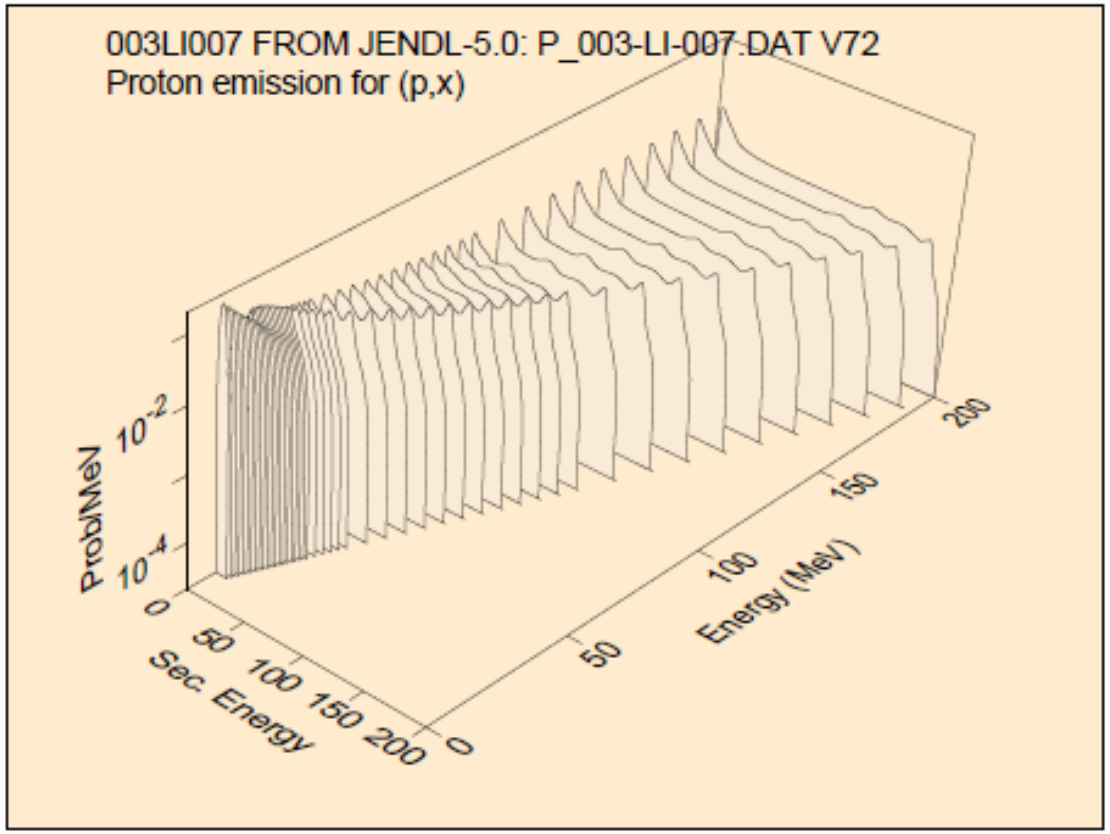
NJOY2016.65 conversion of law7 to law67



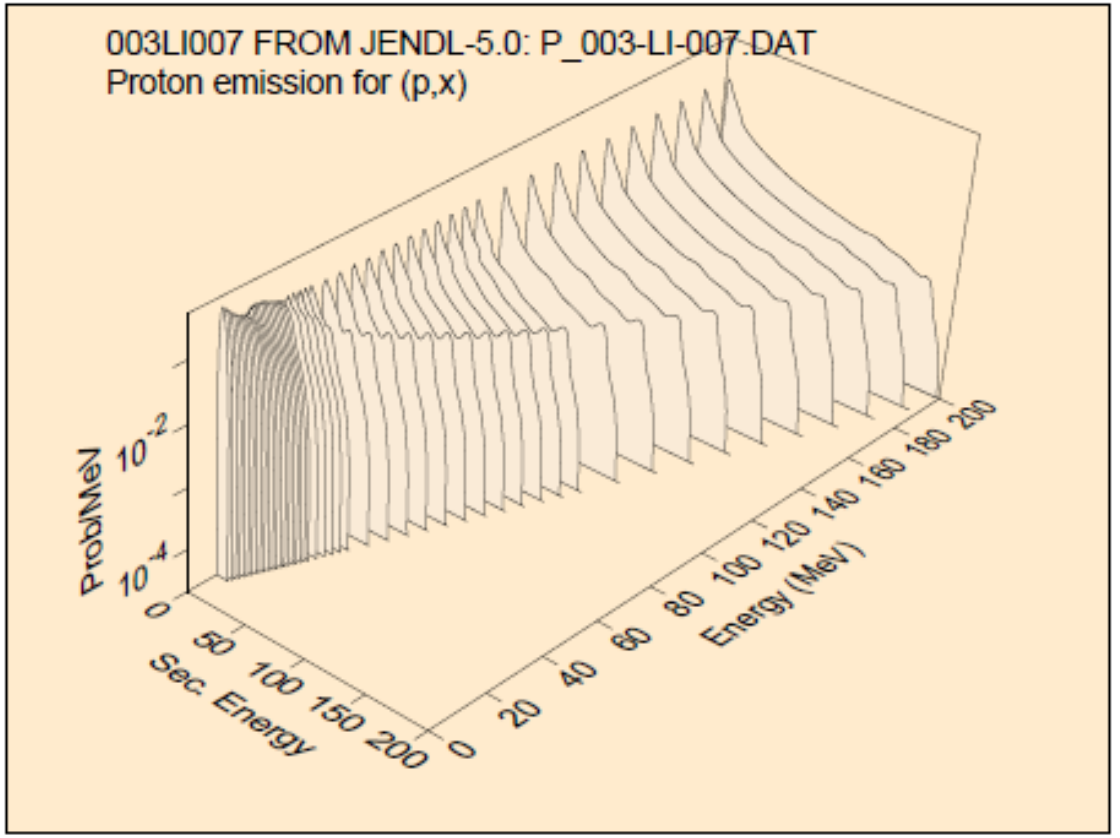
NJOY2016.72 with updates conversion of law7 to law67



NJOY2016.72 conversion of law7 to law61



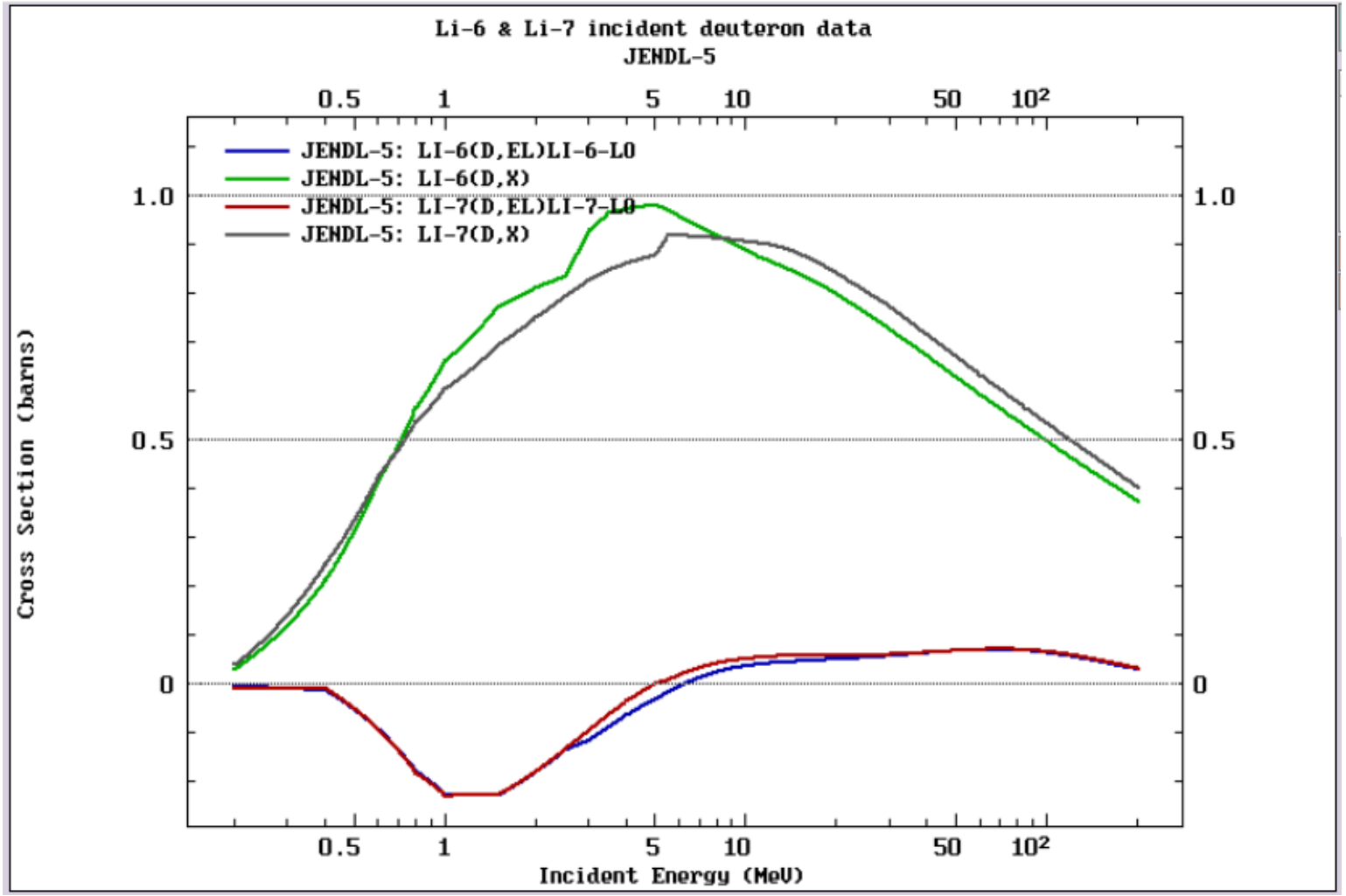
NJOY2016.72 with updates conversion of law7 to law67



Warning: Something to check !!!

?

Elastic cross section uses nuclear + interference representation

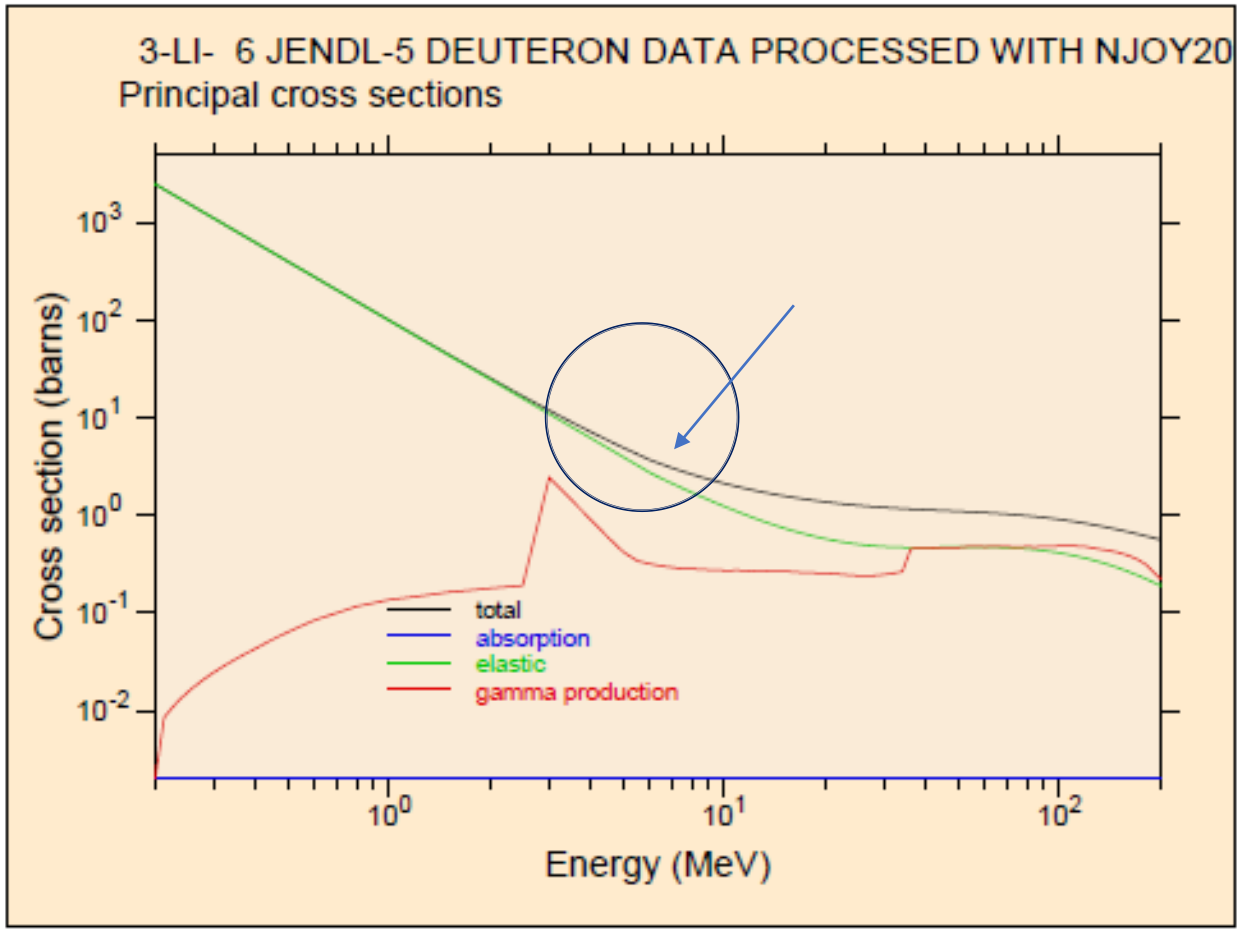


$$\sigma_{NI}(E) = \int_{\mu_{\min}}^{\mu_{\max}} \left[\sigma_e(\mu, E) - \sigma_c(\mu, E)\right] d\mu$$

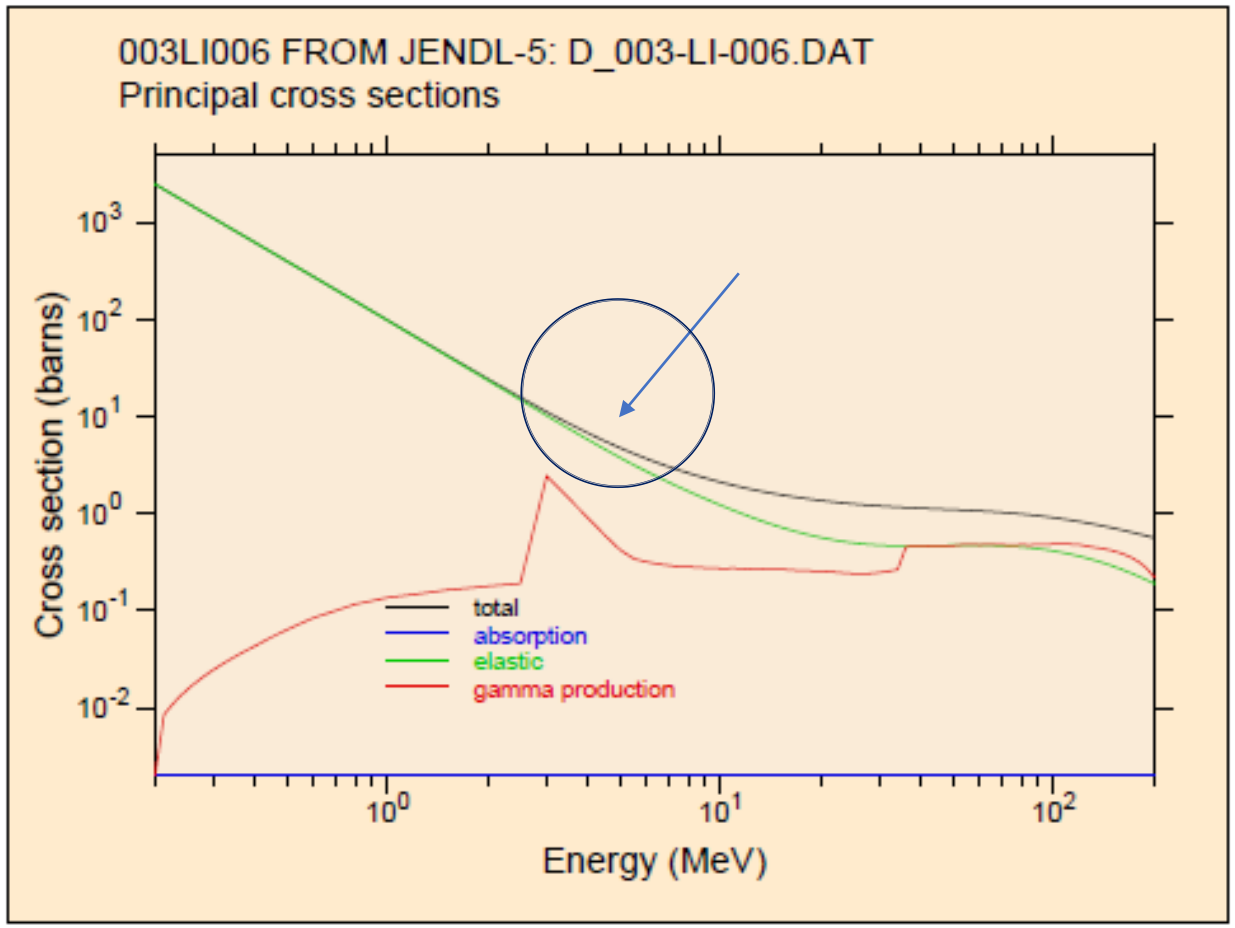
$$P_{NI}(\mu, E) = \begin{cases} \dfrac{\sigma_e(\mu, E) - \sigma_c(\mu, E)}{\sigma_{NI}(E)} & \mu_{\min} \le \mu \le \mu_{\max} \\ 0 & \text{otherwise,} \end{cases}$$

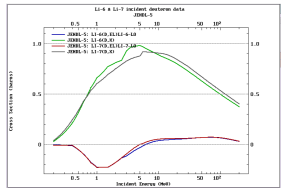
Li-6 Deuteron data

NJOY2016.65/.72 without RECONR/ACER updates



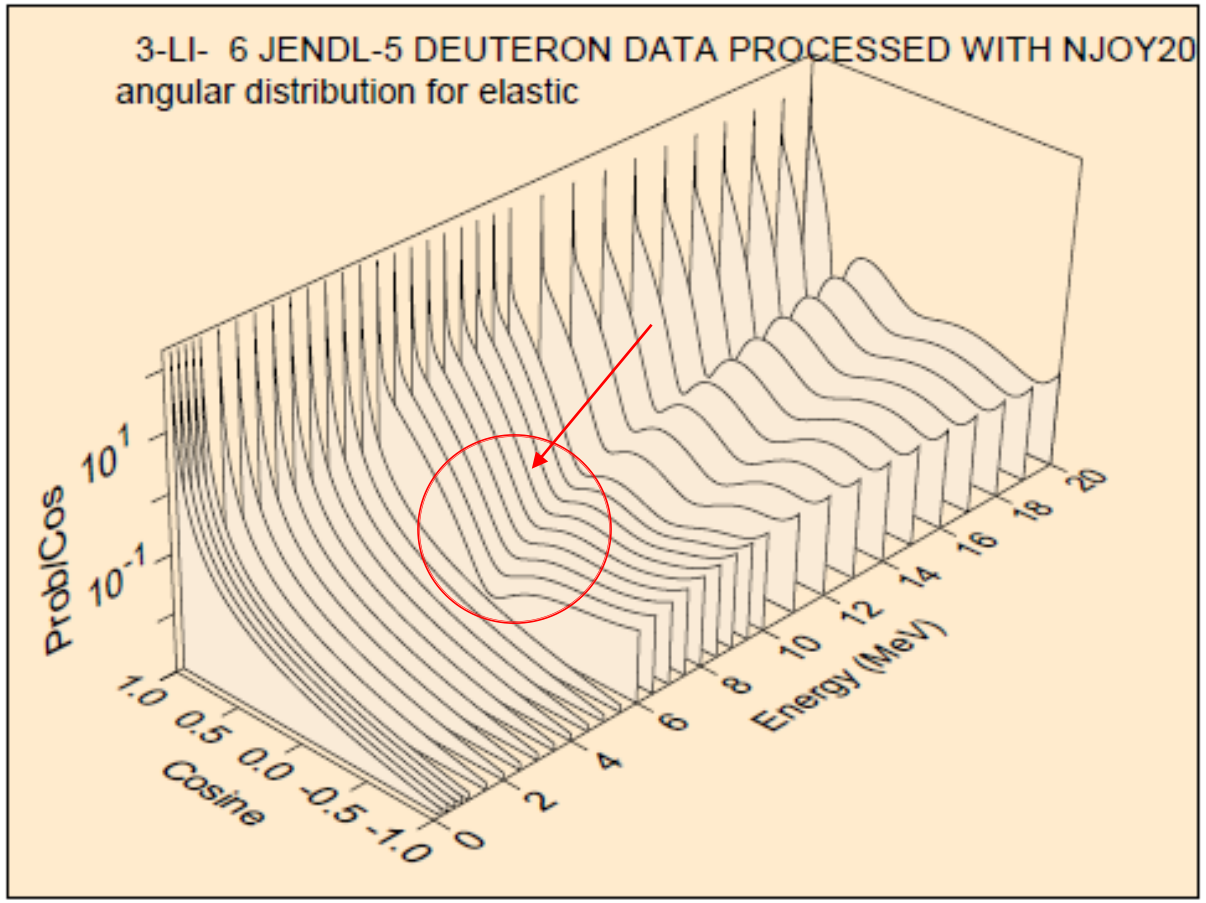
NJOY2016.72 with RECONR/ACER updates



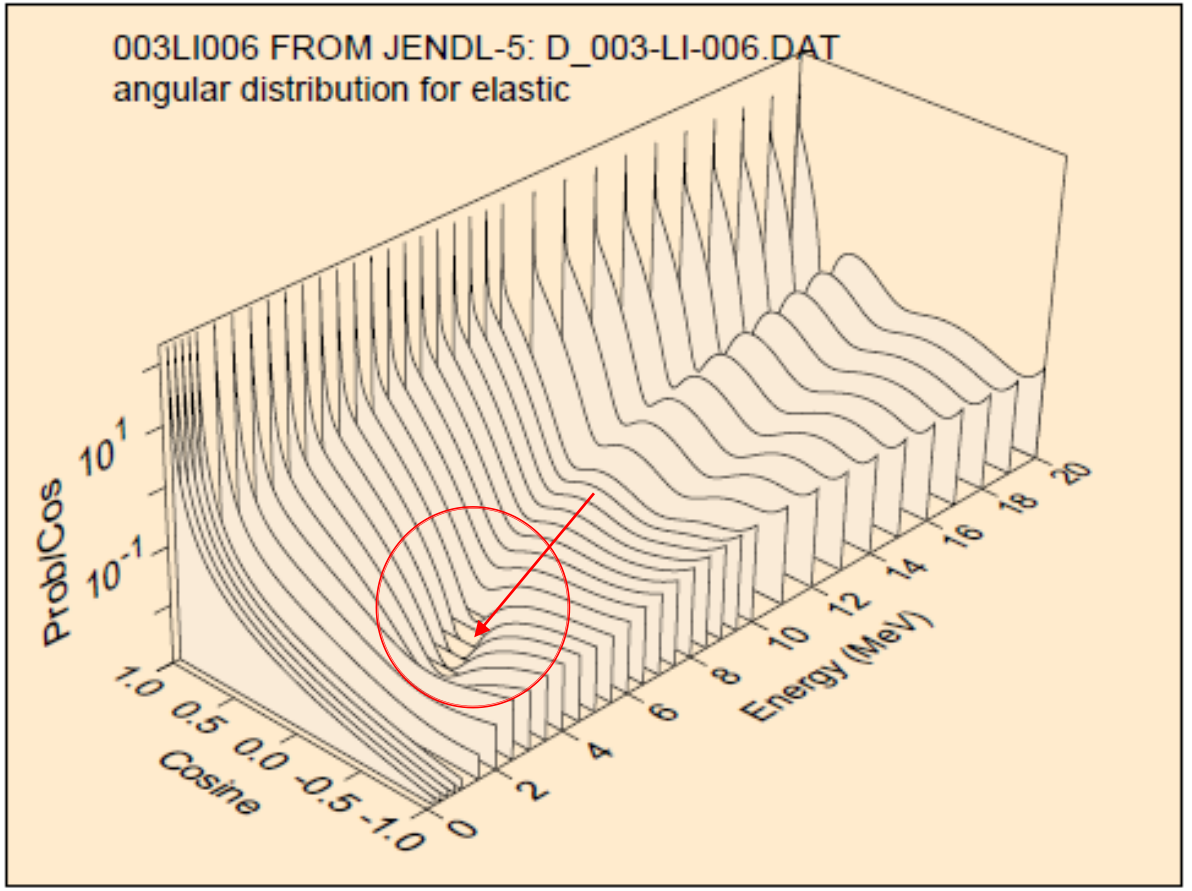


Li-6 Deuteron data

NJOY2016.65/.72 without RECONR/ACER updates



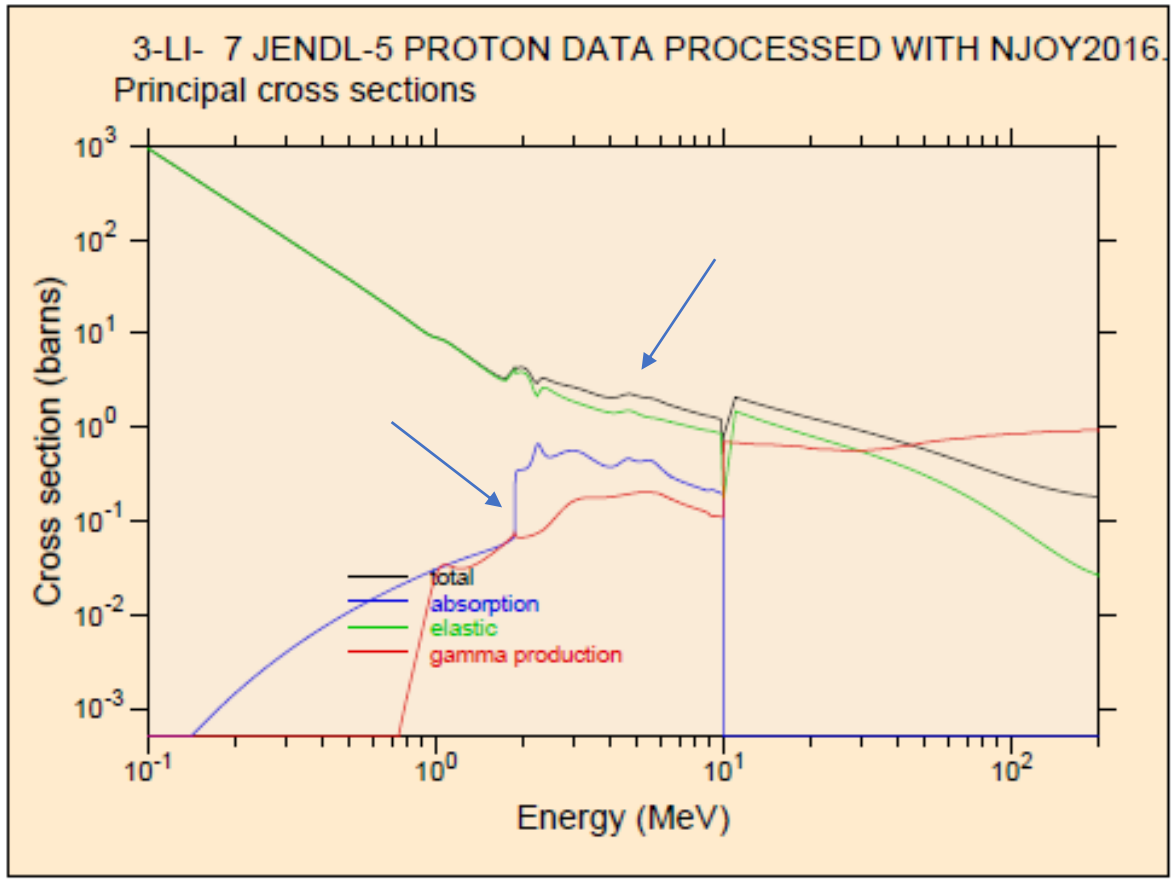
NJOY2016.72 with RECONR/ACER updates



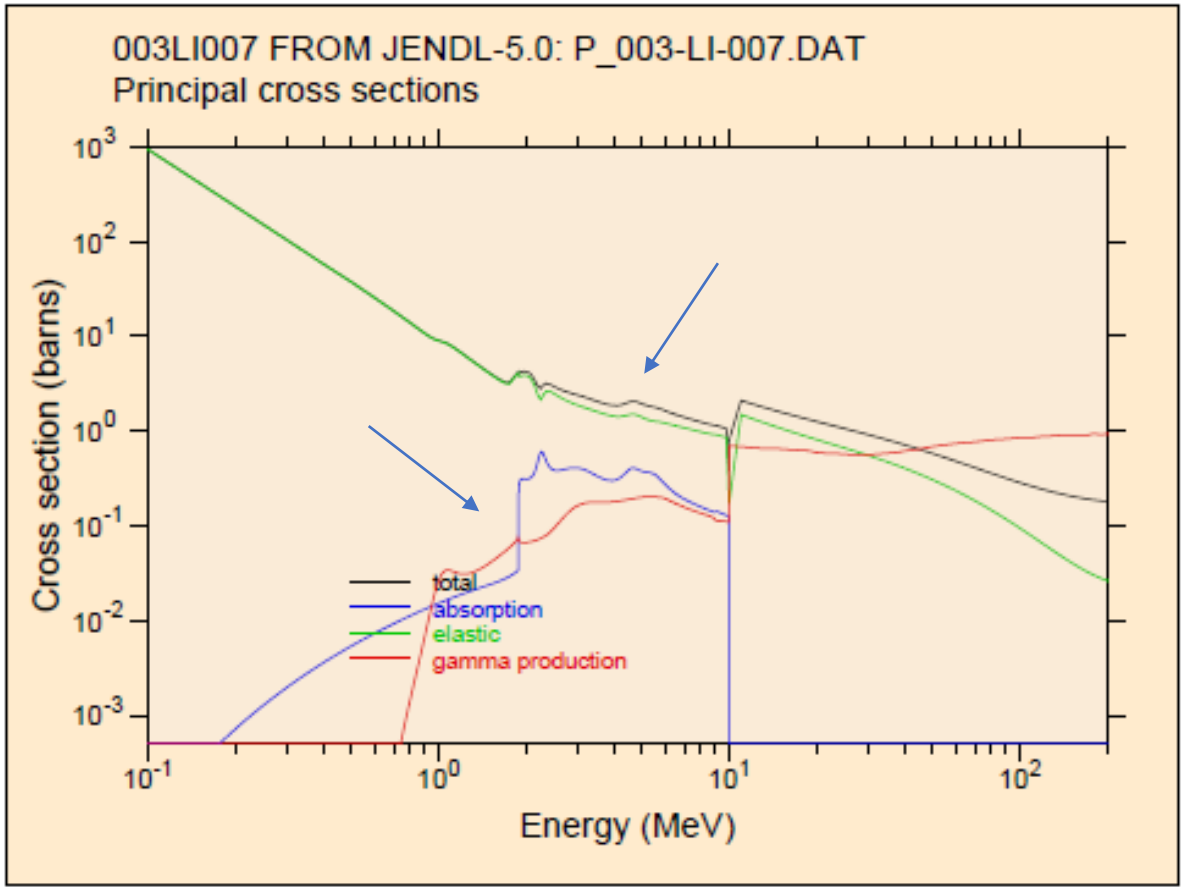
Li-7 incident proton data
Directory data MF/MT=1/451

MF	MT	N	NMOD	MAT	MF/MT	NS
1	451	135	1	328	1451	121
3	2	20	0	328	1451	122
3	5	20	0	328	1451	123
3	50	100	0	328	1451	124
3	51	67	0	328	1451	125
3	601	123	0	328	1451	126
3	650	111	0	328	1451	127
3	800	133	0	328	1451	128
6	2	3495	0	328	1451	129
6	5	194123	0	328	1451	130
6	50	231	0	328	1451	131
6	51	197	0	328	1451	132
6	601	329	0	328	1451	133
6	650	71	0	328	1451	134
6	800	374	0	328	1451	135
				328	1	099999

NJOY2016.65/.72 without RECONR/ACER updates



NJOY2016.72 with RECONR/ACER updates



Li-7 incident protons (ACE files)

NJOY2016.65/.72 without new updates

hk--- 3-Li- 7 JENDL-5 proton data processed with NJOY2016.65.J5

reaction descriptors

reaction	mt	tyr	lsig	land	ldlw	emin	emax	q
elastic	2			1		1.000000E-01	2.000000E+02	
(p,x)	5	101	1	37593	103	9.999990E+00	2.000000E+02	0.000000E+00
inelastic	103	0	51	0	290270	5.447266E-01	2.000000E+02	0.000000E+00
(p,p*1)	601	0	1168	40583	290281	5.477612E-01	2.000000E+02	-4.776120E-01
(p,n)	4	0	2284			2.371167E+00	2.000000E+02	0.000000E+00
(p,n*0)	50	0	3029			1.880451E+00	2.000000E+02	-1.644258E+00
(p,n*1)	51	0	3930			2.371167E+00	2.000000E+02	-2.073338E+00
(p,d)	104	0	4675			5.733333E+00	2.000000E+02	0.000000E+00
(p,a)	107	0	5171			1.000000E-01	2.000000E+02	0.000000E+00
(p,xp)	203	0	6357			5.447266E-01	2.000000E+02	0.000000E+00
(p,xd)	204	0	7474			5.733333E+00	2.000000E+02	0.000000E+00
(p,xt)	205	0	7970			9.999990E+00	2.000000E+02	0.000000E+00
(p,xhe3)	206	0	8020			9.999990E+00	2.000000E+02	0.000000E+00
(p,xa)	207	0	8070			1.000000E-01	2.000000E+02	0.000000E+00
(p,d*0)	650	0	9256			5.749367E+00	2.000000E+02	-5.025447E+00
(p,a*0)	800	0	9751			1.000000E-01	2.000000E+02	1.734724E+01

NJOY2016.72 with new updates

hk---003Li007 from JENDL-5.0: p_003-Li-007.dat

reaction descriptors

reaction	mt	tyr	lsig	land	ldlw	emin	emax	q
elastic	2			1		1.000000E-01	2.000000E+02	
(p,x)	5	101	1	37593	103	9.999990E+00	2.000000E+02	0.000000E+00
(p,p*1)	601	0	52	40583	290270	5.477612E-01	2.000000E+02	-4.776120E-01
(p,n*0)	50	0	1169			1.880451E+00	2.000000E+02	-1.644258E+00
(p,n*1)	51	0	2071			2.371167E+00	2.000000E+02	-2.073338E+00
(p,d*0)	650	0	2817			5.749367E+00	2.000000E+02	-5.025447E+00
(p,a*0)	800	0	3313			1.000000E-01	2.000000E+02	1.734724E+01

1-H-2 for incident protons from JENDL-5: Use of MF6/law6 N-body phase-space

Directory MF1/MT451

```
1          451          103           1 128 1451    96
3            2           19           0 128 1451    97
3            3           38           0 128 1451    98
3            5           38           0 128 1451    99
3           28           42           0 128 1451   100
6            2         1463           0 128 1451   101
6            5           80           0 128 1451   102
6           28            9           0 128 1451   103
                                        128 1  099999
```

Warning!!!

NJOY2016 assumed Center of Mass System (CM)

I just added a warning for the time being

1. Final comments

Energy-angle distributions MF6/MT28 1-H-2(p,np)1-H-1

```
1.002000+3 1.997000+0          0           1          2          0 128 6 28    1
1.000000+0 1.000000+0          0           6          1          2 128 6 28    2
         2          2                                             128 6 28    3
3.339002+6 1.000000+0 2.000000+8 1.000000+0                       128 6 28    4
2.995620+0 0.000000+0          0           0          0          3 128 6 28    5
1.001000+3 9.986200-1          0           6          1          2 128 6 28    6
         2          2                                             128 6 28    7
3.339002+6 2.000000+0 2.000000+8 2.000000+0                       128 6 28    8
2.995620+0 0.000000+0          0           0          0          3 128 6 28    9
                                                                  128 6  099999
```

Laboratory reference system (LAB)

endf/mf6/law6: N-Body phase space

c:\NJOY2016-2016.72\src\acefc.f90 >> d:\NJOY2016\src\acefc.f90

Compare | Next difference | Previous difference | Font | Binary | Case sensitive

Edit mode | Show only differences, with extra lines: 1 | ANSI<->ANSI | Ignore repeated spaces | Ignore frequent lines

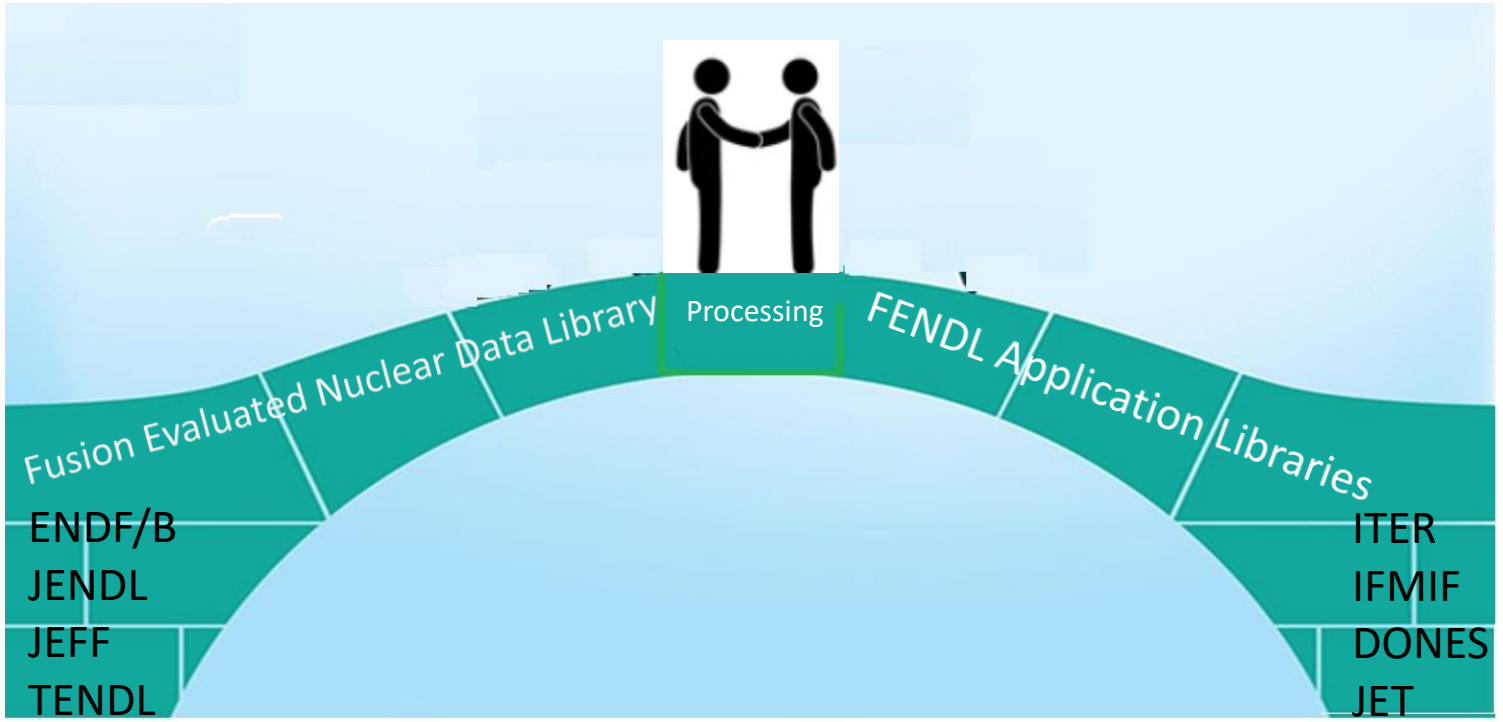
```
7678:          !--process according to lang
7679:
7680:          !--distribution given in kalbach format
7681:          if (lang.eq.2) then
7682:             xss(ki+3*n+nexd)=scr(9+ncyc*(ki-1))
7683:             if (na.eq.2) then
7684:                aa=scr(10+ncyc*(ki-1))
7685:             else
7686:                aa=bachaa(1,1,iza,ee,ep)
7687:             endif
7688:             xss(ki+4*n+nexd)=sigfig(aa,7,0)
7689:
7690:          !--convert legendre distribution to kalbach form
7691:          else if (lang.eq.1.and.newfor.ne.1) then
7692:             iso=1
7693:             do ik3=1,na
7694:                if (scr(8+ik3+ncyc*(ki-1)).ne.zero) iso=0
7695:             enddo
7696:             if (bzro.eq.0.) iso=1
```

```
7853:          !--process according to lang
7854:
7855:          !--distribution given in kalbach format
7856:          if (lang.eq.2) then
7857:             xss(ki+3*n+nexd)=scr(9+ncyc*(ki-1))
7858:             if (na.eq.2) then
7859:                aa=scr(10+ncyc*(ki-1))
7860:             else
7861:                aa=bachaa(izai,nint(zap),iza,ee,ep)
7862:             endif
7863:             xss(ki+4*n+nexd)=sigfig(aa,7,0)
7864:
7865:          !--convert legendre distribution to kalbach form
7866:          else if (lang.eq.1.and.newfor.ne.1) then
7867:             iso=1
7868:             do ik3=1,na
7869:                if (scr(8+ik3+ncyc*(ki-1)).ne.zero) iso=0
7870:             enddo
7871:             if (bzro.eq.0.) iso=1
```

3. Final comments

- A set of updates were developed for processing FENDL using the latest version of NJOY2016
- The impact is expected in heating numbers and damage cross sections for neutrons and in the protons and deuteron continuous energy ACE-formatted files
- The proposed updates have been sent to NJOY developers at LANL for reviewing
- NJOY2016.72+updates available on https://github.com/IAEA-NDS/NJOY2016
- More verification and validation of processing methods is required

Thank you!


Fusion Evaluated Nuclear Data Library
Processing
FENDL Application Libraries
ENDF/B
JENDL
JEFF
TENDL
ITER
IFMIF
DONES
JET