

Nuclear data processing codes and steps - a primer

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Preliminary comments

Nuclear observables, data forms needed for engineer, practitioner are not always the same as the ones needed by evaluator

Processed files useful for application(s) are not anymore ENDF-6 format compliant, similar maybe, derived certainly

Processed nuclear data forms are numerous, rich, abundant, diverse. Some are observable other not; all have a specific importance for at least one applications

Processing enhances, enriches, deepens the evaluated nuclear data forms

Lexical semantics

Global Nuclear Data Structure: GNDS
Evaluated Nuclear Data Format: ENDF-6

} Format

Hybrid END File >> from PREPRO to JANIS, ZvView, FISPACT-II,..

Pointwise END File >> from NJOY, PREPRO, CALENDF,...to many codes

Groupwise END File, Matrices >> from NJOY, PREPRO, AMPX... to many codes

ANISOTropy >> from TRIPOLI-4 to TRIPOLI-4

A Compact Endf >> from ACER, FRENDY, FUDGE... to MCNP, SERPENT, OpenMC,...

Probability Tables >> from CALENDF, PURR... to FISPACT-II, MCNP, TRIPOLI,...

PDF, CDF, TF >> from NJOY, PREPRO to MCNP, SERPENT, OpenMC, TART,...

.....

It is important to differentiate between:

3 | format and formalism, nuclear data forms

Lexical semantics

- Hybrid END File
- Pointwise END File
- Groupwise END File
- ANISOtropy
- A Compact Endf
- Probability Tables
- PDF and CDF
- ...

Nuclear data forms

Formalisms

- Multi-Level-Breit-Wigner, Reich-Moore, R-Matrix Limited, Legendre, Blatt and Biedenharn, Kalbach-Mann, Froehner, Watt,...

Lexical semantics

Pre-processing steps: convert the ENDF-6 nuclear data into **simple forms** that can be interpreted

Processing steps: processes the ENDF-6 nuclear data into **complex forms** useful for applications: particles transport, reactor analysis codes, inventory, source terms, etc.

Post-processing steps: verify either of the above steps

The lexical is ancient, as the 'tape' the above usually modular and sequential steps I/O uses. It belongs to the dawn of the computer age, does sound a bit odd now a day, however it still works – just about

if it ain't broke, don't fix it

ENDF-6 Format Manual

De facto the standard

Files 1-10 n-description, also p, d, α , γ -induced

Files 11-15 γ -description

Files 23-28 atomic data

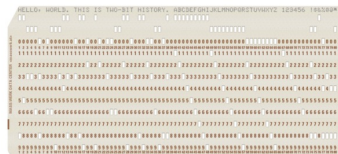
Files 30-40 covariance description

431 pages; **dusty & clutter & rune**

Most of the World libraries are distributed in that format

Designed, crafted by evaluator and engineer with science, application in mind, since May 1966 – **half a century ago !!**

6 |



CSEWG Document ENDF-102
Report BNL-224854-2023-INRE
Git Revision SHA1: 3576914



ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
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Generalised Nuclear Database Structure (GNDS)

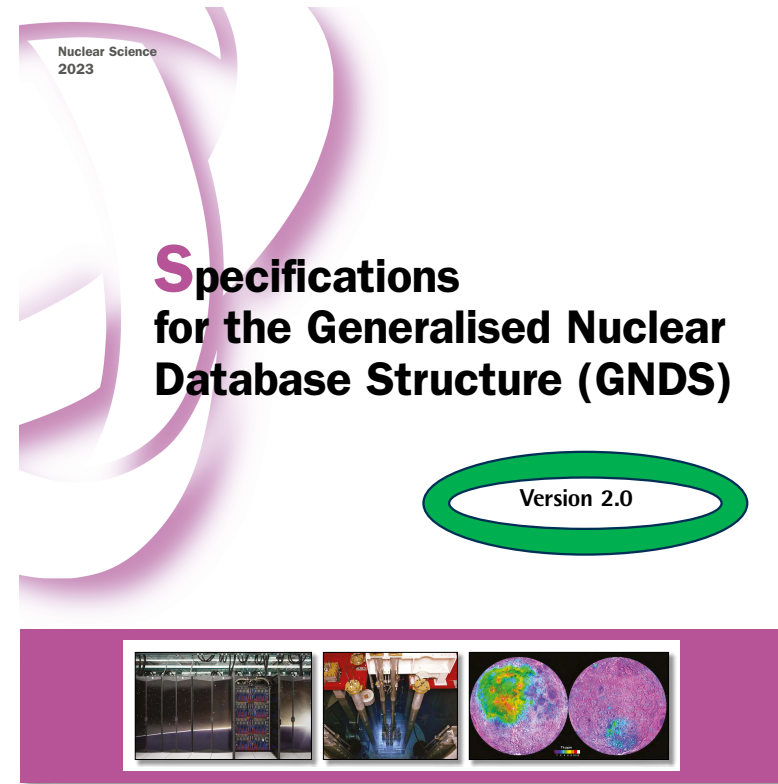
The new standard

A modern structure not a format

435 pages

Some of the World libraries are now distributed in that format, **slow to take over**

Designed, crafted by practitioner with science and Multiphysics in mind, born with the millennia to unleash simulation's potentials



Processing codes & steps & practices

ENDF file

- **NJOY-2016**

- reconr
- broadr
- unresr
- **thermr**
- **heatr**
- **gaspr**
- **mixr**
- **purr**
- **acer**
- **groupr**

cross-check



- **PREPRO-2023**

- linear
- recent
- sigma1
- **legend**
- **sixpack**
- **spectra**
- **activate**
- **merger**
- **fixup**
- **dictin**

cross-check



- **CALENDF**

- **FRENDY**
- **AMPX**
- **GALILEE**
- **FUDGE**
- **NECP-Atlas**
- **NDEX**
- ...

Single script,
many steps for
an entire library

PENDF file

ACE file

Hybrid file

NJOY Processing scripts

1 basics & isotopic

```

cat>in$isma[$c1] <<EOF
moder
20 -21/ -- moder check & mode
reconr
-21 -22
'pendf $isma[$c1] ENDF/B-VIII.1 '
$isma[$c2]/
.001/
0/
moder
-22 36/ -- pendf OK
broadr
-21 -22 -23
$isma[$c2] 1/
.001/
293.6/
0/
unresr
-21 -23 -24
$isma[$c2] 1 1 0/
293.6/
1.e+10/
0/
moder
-24 32/ -- pendf 293.6K sig-0 & T4XS
heatr
-21 -24 -26 30
$isma[$c2] 7 0 0 1 2/ -- heatr gamma heat local & chk print
302 303 304 318 401 403 407/
heatr
-21 -26 -27 33
$isma[$c2] 6 0 0 1 2/
442 443 444 445 446 447/
gaspr
-21 -27 -29
moder
-29 35/ -- pendf 293.6K & gas mt20x, partials mt30x kermas & mt40x damages
viewr
30 31/ -- viewr energy-balance check

```

```

cat>in$isma[$c1] <<EOF
moder
20 -21/ -- moder check & njoy mode
thermr
0 -22 -23
0 $isma[$c2] 20 1 1 0 0 1 221 0/ -- thermr free gas
293.6 /
0.001 10./
purr
-21 -23 -24
$isma[$c2] 1 1 20 64 / -- purr sig-0 20 bins 64 ladders
293.6 /
1.e+10/
0 /
-- heatr overwrite with gamma transported
heatr
-21 -24 -25 29
$isma[$c2] 7 0 0 0 2/
302 303 304 318 401 442 443/
heatr
-21 -25 -26 30
$isma[$c2] 4 0 0 0 2/
444 445 446 447/
--
-- 1st acer fast
acer
-21 -26 0 32 33/
1 1 1 0.81 0/
'Ace $isma[$c1] ENDF/B-VIII.1'
$isma[$c2] 293.6/
1 1/
/

```

2 ace & other

```

--
-- 2nd acer check/plot/correct
acer
0 32 34 35 36/
7 1 1 -1/
'Ace $isma[$c1] ENDF/B-VIII.1 - check 1'
-- tape35 ACE file, tape36 xmdir
-- pendf for Ace 293.6K &
-- mt152 bondarenko unresolved
-- mt153 probability tables unresolved
-- mt221 free gas thermal scattering
-- mt20x gaz production
-- mt30x partials kermas
-- mt40x partials damages
viewr
30 31/ -- heatr gamma heat nonlocal & chk print
viewr
34 37/ -- acer plots check 1
moder
-26 38/ -- pendf ace
stop

```

NJOY Print options: 0, 1, 2

A plethora of usually untapped information, intermediary and final forms, numerical and graphical outputs: **Verification** processes

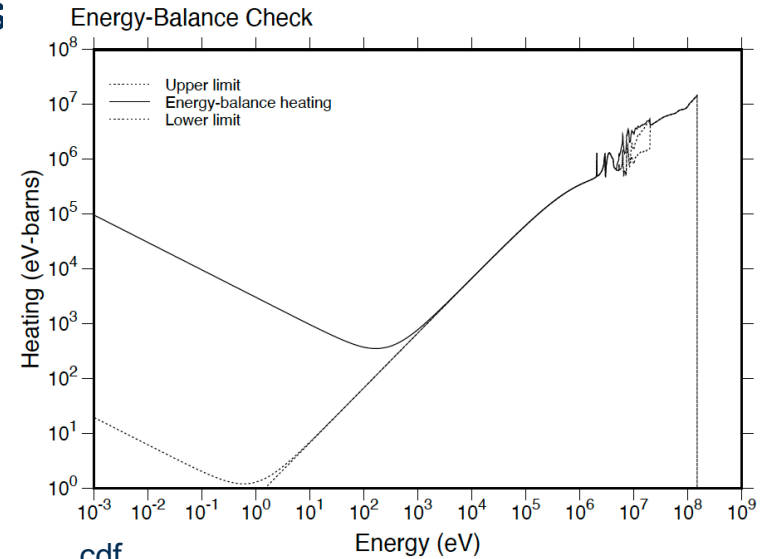
broadr, heatr, acer, groupr,....

thermal quantities at **293.6 K = 0.0253 eV**

 thermal capture xsec: 3.8620E-03
 thermal capture integral: 3.4230E-03
 capture resonance integral: 2.0556E-03

angular distributions for
 incident particle energy = 2.000000E+00 int = 2 np = 18

cosine	pdf	cdf	cosine	pdf	cdf
-1.000000E+00	6.333382E-01	0.000000E+00	-9.210000E-01	5.802944E-01	4.793849E-02
-8.430000E-01	5.368052E-01	9.150538E-02	-7.650000E-01	5.014318E-01	1.319966E-01
-6.870000E-01	4.734805E-01	1.700182E-01	-6.090000E-01	4.522744E-01	2.061226E-01
-5.310000E-01	4.371543E-01	2.408103E-01	-4.520000E-01	4.273886E-01	2.749597E-01
-3.590000E-01	4.221798E-01	3.144646E-01	-2.810000E-01	4.223566E-01	3.474015E-01
-1.870000E-01	4.272212E-01	3.873317E-01	-6.250000E-02	4.399583E-01	4.413136E-01
6.250000E-02	4.580496E-01	4.974392E-01	3.130000E-01	5.026719E-01	6.177696E-01
5.630000E-01	5.472430E-01	7.490090E-01	7.500000E-01	5.738266E-01	8.538290E-01
9.070000E-01	5.884447E-01	9.450673E-01	1.000000E+00	5.929042E-01	1.000000E+00



Look at the output

NJOY output files

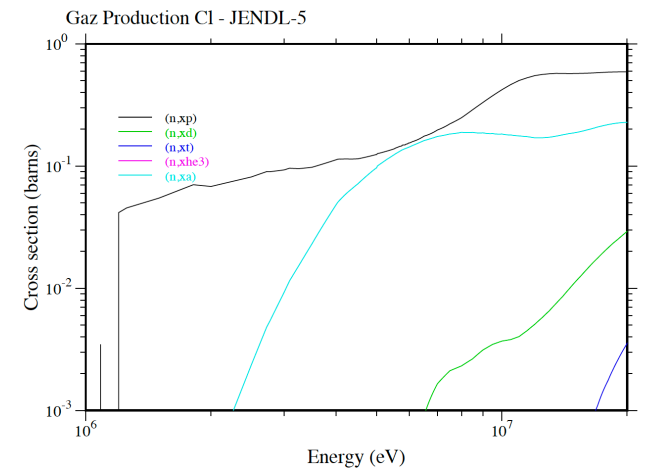
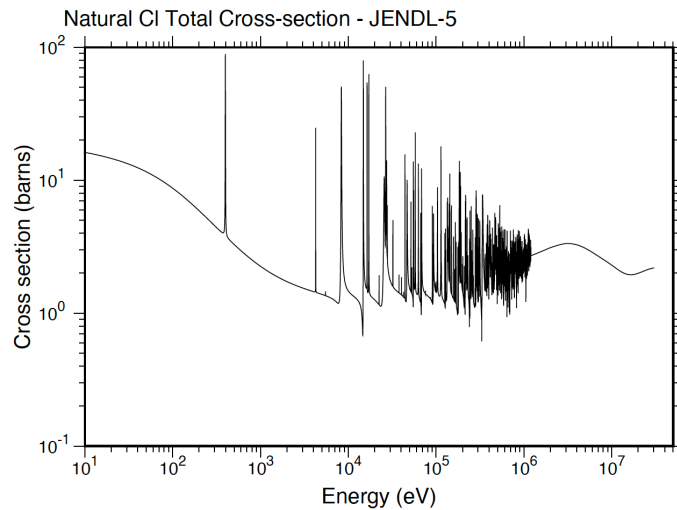
Processing scripts to natural target

NJOY-2016 mixr & plotr & viewr

- Any MF=1-3 MT's + derived mts
- DPCS mts= 444 - 447
- KERMA mts= 301- 450
- GAZ production mts= 203 - 205

```

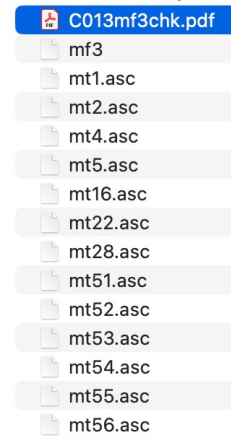
cat>in$zant[$c1] <<EOF
mixr
30 $tx/
1 203 204 205 206 207 301 442 443 444 445 446 447/
$mx/
293.6/
$zant[$c2] $zant[$c5] $zant[$c3]/
'$zant[$c4]-$zant[$c1]- 0 IAEA TENDL-2024 $zant[$c1] Natural'/
plotr
31/
/
1/
'Natural $zant[$c1] Total Cross-section - TENDL-2024'/
/
4/
1e+1 3.e7/
/
/
6 30 $zant[$c2] 3 1 293.6/
0 0 0 0 1/
99/
viewr
31 32
stop
    
```



```

# In -sf ../Orig/n-$isma[$c1].tendl tape20 # ENDF-6 raw
# In -sf ../pendf/$isma[$c1]p.asc tape20 # NJOY2016 pendl, only mf3
# In -sf ../pendf-red/pendf/$isma[$c1]p.asc tape20 # PREPRO pendl mf3 & mf10
#
# mkdir $isma[$c1] # X-Y tables directory
#
# grep "          3          " tape20 | cut -c 42-44 > mf3 # List all MT in MF3
#
set ismts = (`cat mf3`)
#
set nbrmtd = $#ismts
set count1 = 1
set c3 = 1
#
while ($count1 <= $nbrmtd)
#
echo 'running njoy'
cat>in$isma[$c1] <<EOF
plotr
31/
/
1/
'$isma[$c1] mt = $ismts[$c3]/
/
/
/
/
/
/
/
6 20 $isma[$c2] 3 $ismts[$c3] 293.6/ iverf nin matd mfd mtd temper nth,ntp,nkh
/
99/
stop

```

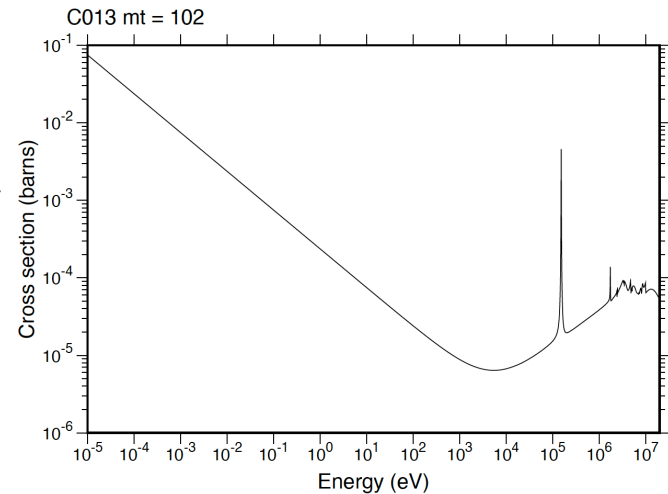


pdf book

```

viewr
31 32
stop
EOF
/opt/Code/NJOY2016/build/njoy<in$isma[$c1]
echo 'saving output files'
ps2pdf14 tape32
mv tape32.pdf $isma[$c1]/mt$ismts[$c3].pdf
mv tape31 $isma[$c1]/mt$ismts[$c3].asc
rm output
rm in$isma[$c1]
#
@ count1++
@ c3+=1
end
pdftk $isma[$c1]/*.pdf cat output $isma[$c1]/$isma[$c1]mf3chk.pdf
rm $isma[$c1]/mt*.pdf
rm tape*
mv mf3 $isma[$c1]/mf3
@ count++
@ c1+=2
@ c2+=2
end

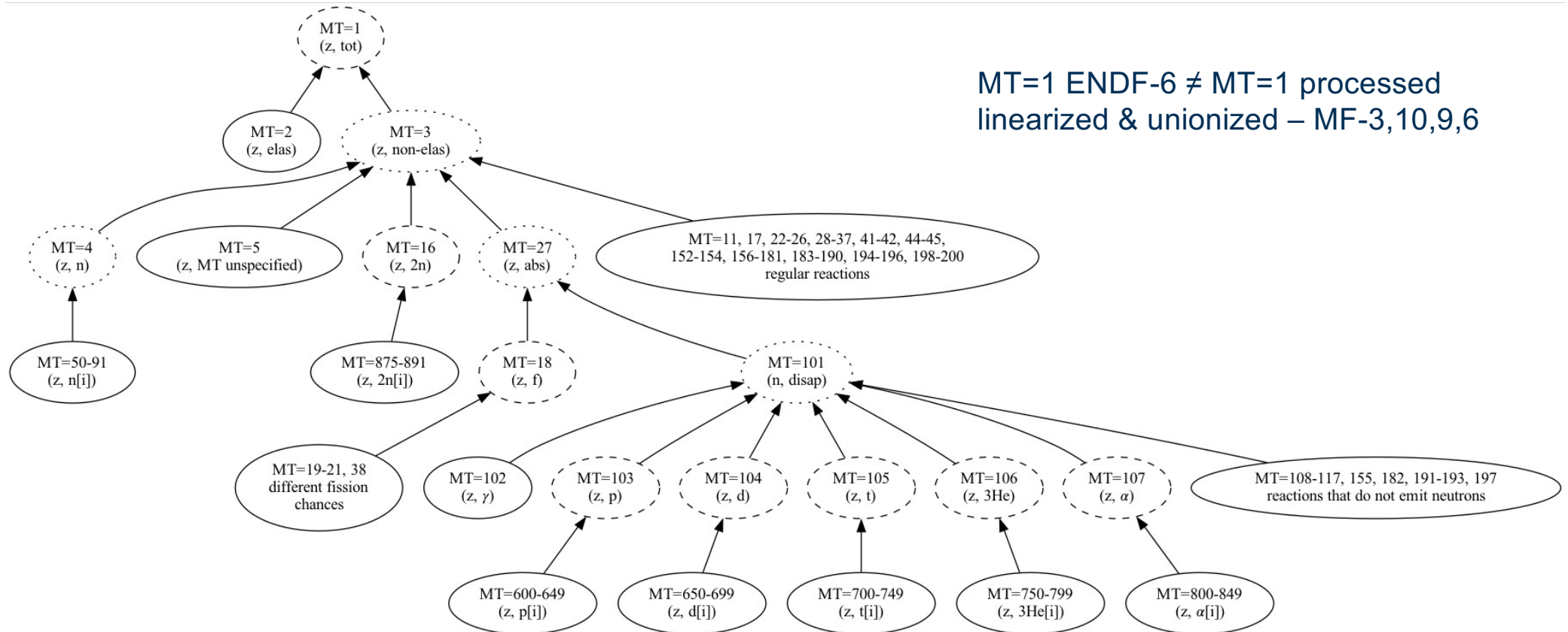
```



Thinned XS, X-Y 2 columns
ready for plotting, <10000 pts

Processing delicacy: ENDF-6 sum rules

Incomplete when explicit, with grey areas: TSL, MF-2 open channels,...

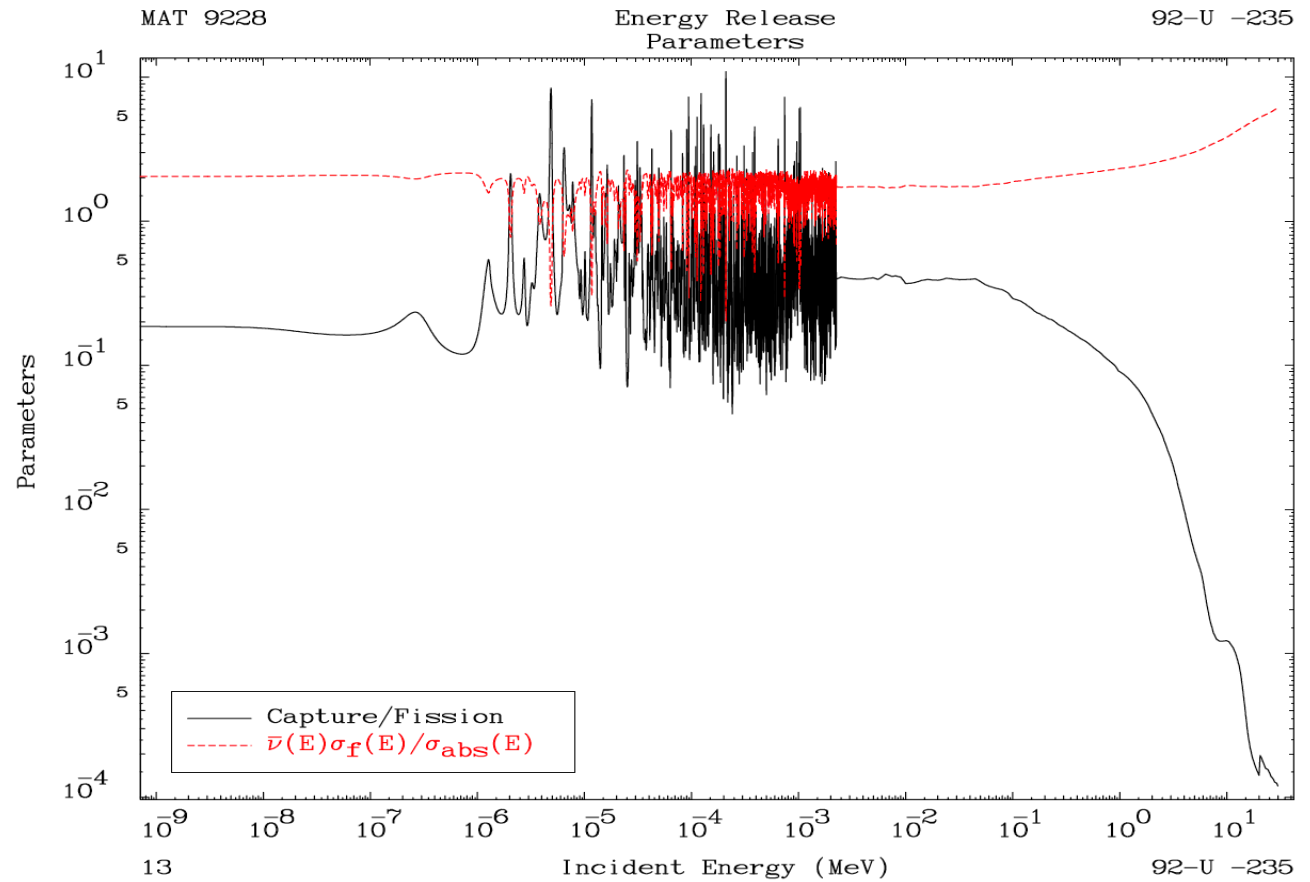
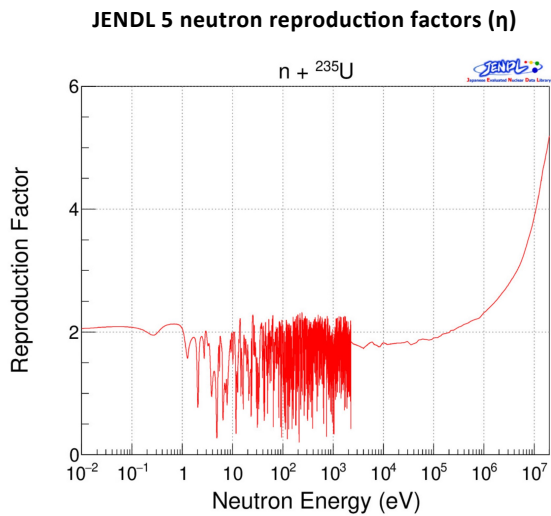


Processing scripts PREPRO fixup

PREPRO fixup can fix many things !! had to

```
cat>FIXUP.INP <<EOF
10001111111000
../pendf/$isma[$c1]p.asc
FIXUP.OUT
  27=( 18, 18)+(102,117)
*333=(452* 18)
R255=(333/ 27)
R254=(102/ 18)
*****
```

EOF



Processed data forms

Sorted by: [Reactions] Reorder by: [Libraries] View: basic extended: get MAT, PEN, GND, run Inter: resonance integrals, etc.

1) MN-55 (N, TOT), SIG MT=1 MF=3 NSUB=10

MF3: [SIG] Cross sections MT1: [N, TOT] Neutron total cross sections.

1 **MAT** **GND-1.2** **PEN** **Inter** **Info** **Summary** **ENDF-6** **Interpreted** **js** **MF3-Plot** **Plot** JENDL-5 E=200MeV Lab=JAEA Date=20210607 N. Iwamoto

```
PROGRAM INTER VERSION 6.00
Selected integrations of ENDF file 3 and file 10 cross sections
Thermal cross section : Sig(220) = Sig(Eth)
Thermal energy (eV) : Eth = 2.53500E-02 (eV)
Macro cross section : Sig(Ezero)
Macro energy (eV) : E0 = 2.53500E-02 (eV)
Maxwellian average : Avg-Sigma = 2*sqrt(Pi) / Intg(E1(E2) Sig(E1) PHL_M(E) dE / Intg(E1(E2) PHL_M(E) dE)
Maxwellian spectrum : PHL_M(E) = 10*(E**2) exp(-E/2)
Spectrum Temperature : kT = 2.53500E-02 (eV)
Integration limits : E1 = 1.00000E-01 (eV) E2 = 1.00000E+01 (eV)
Integral of Spectrum : = 1.00000E+00
Weighted q-factor : Q-Fact = 2*sqrt(Pi) Avg-Sigma / Sig(220)
Resonance Integral : Res Integ = Intg(E1(E2) Sig(E) dE
Integration limits : E1 = 1.00000E-01 (eV) E2 = 1.00000E+05 (eV)
Integral of Spectrum : = 1.00000E+00
Flux Spectral Average : Sig(Fix) = Intg(E1(E2) Sig(E) PHL_Fix(E) dE / Intg(E1(E2) PHL_Fix(E) dE)
Fluxion spectrum : PHL_Fix(E) = sqrt(2/PI) / (E**2 exp(-E/2))
Spectrum Temperature : kT = 1.00000E+01 (eV)
Integration limits : E1 = 1.00000E-01 (eV) E2 = 2.00000E+07 (eV)
Integral of Spectrum : = 1.00000E+00
E14 cross-section : Sig(E14)
Delayed Energy : E14 = 1.00000E+07 eV
```

```
#LIBRARY JENDL-5
#REACTION MN-55 (N, TOT), SIG
#NUCLEUS Mn-55
#MF 3
#MT 1
#EN-MIN 1e-05
#EN-MAX 2e+08
#E, eV Sig, b Interpolation
1E-05 684.49 Lin-Lin
1.10304E-05 651.749 Lin-Lin
1.21669E-05 620.575 Lin-Lin
1.34206E-05 590.893 Lin-Lin
1.48034E-05 562.632 Lin-Lin
1.63286E-05 535.724 Lin-Lin
1.80111E-05 510.104 Lin-Lin
1.98669E-05 485.711 Lin-Lin
2.19139E-05 462.486 Lin-Lin
```

PEN

PREPRO PEN

linear
recent
sigma1
fixup
legend
sixtab ??



IAEA local MF-6 conversion into pointwise in lab with caveats:

- Legendre, Tab. only
- n-incident only
- CM for n only

activate?
spectra?
sixpack ?

Interpreted ENDF file

MN-55(N,TOT),SIG ZA=25055 LISO=0 MAT=2525 MF=3 MT=1 Library: JENDL-5

total cross section

Interpolation table:

1096	2	1136	5
------	---	------	---

Cross section table:

eV	barns	eV	barns	eV	barns
1.00000E-05	0.00000E+0	2.53000E-02	0.00000E+0	1.00000E+0	0.00000E+0
5.00000E+0	9.00000E-3	1.00000E+1	1.10000E-2	3.00000E+1	2.40000E-2
6.00000E+1	2.80000E-2	1.00000E+2	3.30000E-2	2.00000E+2	3.90000E-2
4.00000E+2	3.55000E-2	8.00000E+2	3.10000E-2	3.15000E+3	1.26000E-2

ENDF Web Retrieval System

Conversion ENDF file to GND format.

Request #17769.

MAT: Library="JENDL-5" Target="MN-55" MAT=2525 NSUB=10 (N)

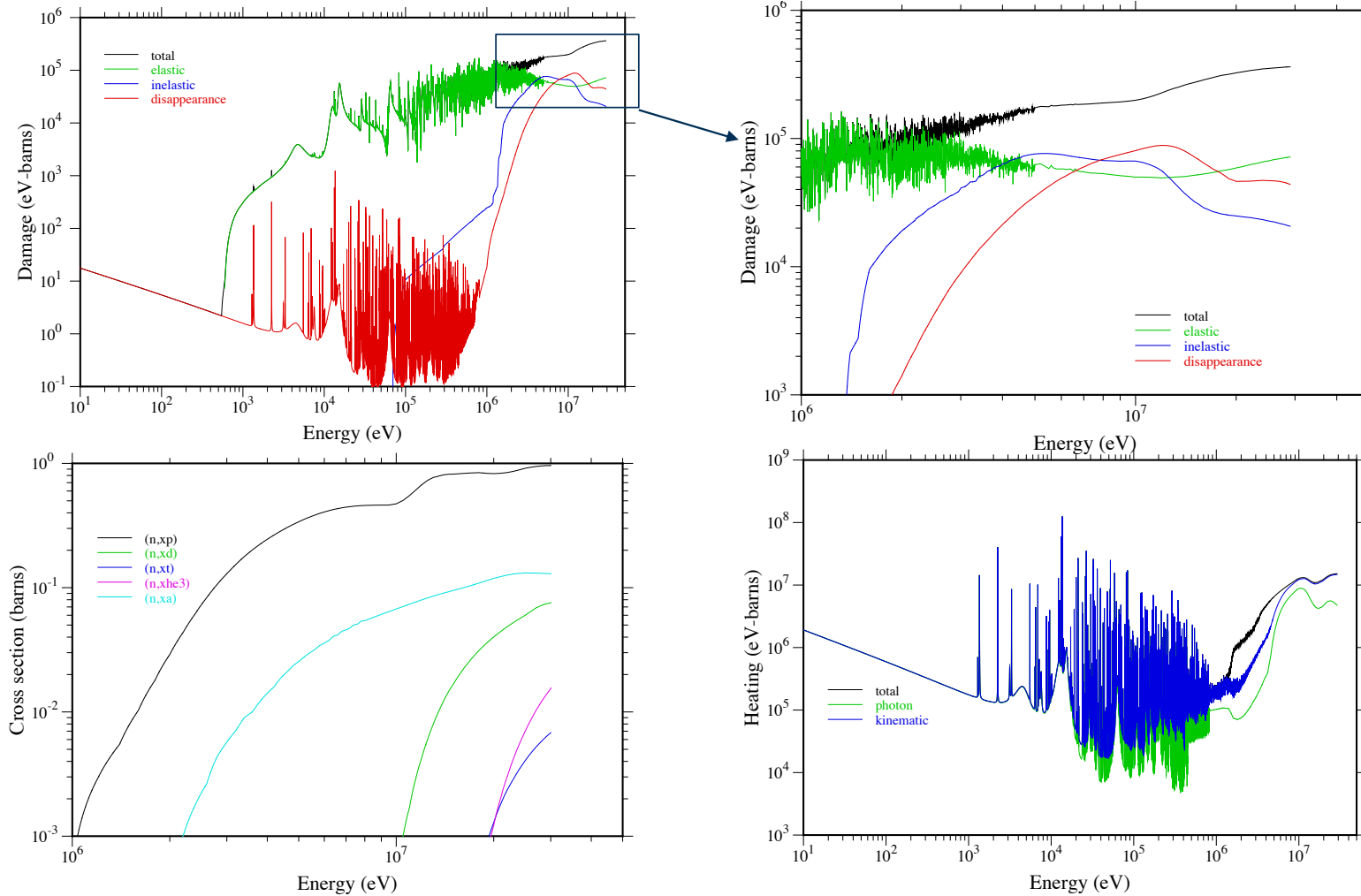
#	File	Comment	Date	Length
1	gnd.endf	Input file	2024/11/06 13:27:40	30,110,697
2	gnd_cmd.err	Error file	2024/11/06 13:27:40	55
3	gnd_cmd.log	Log file	2024/11/06 13:27:40	130
4	gnd_cmd.ttout	Terminal output	2024/11/06 13:27:40	0

---ERROR---

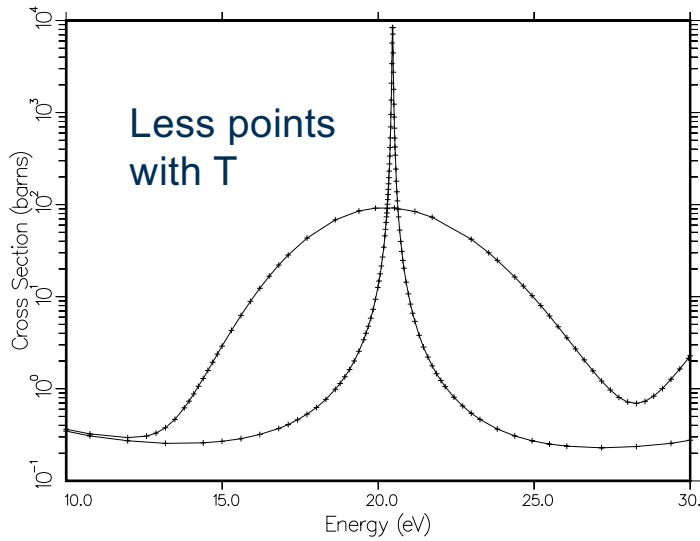
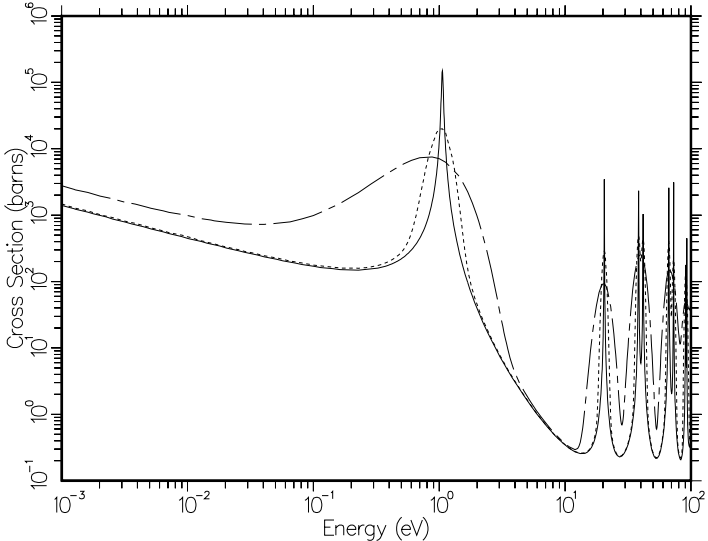
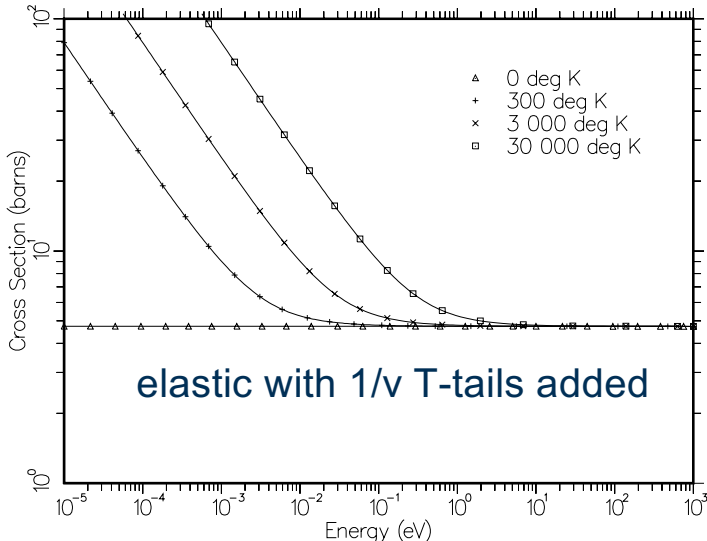
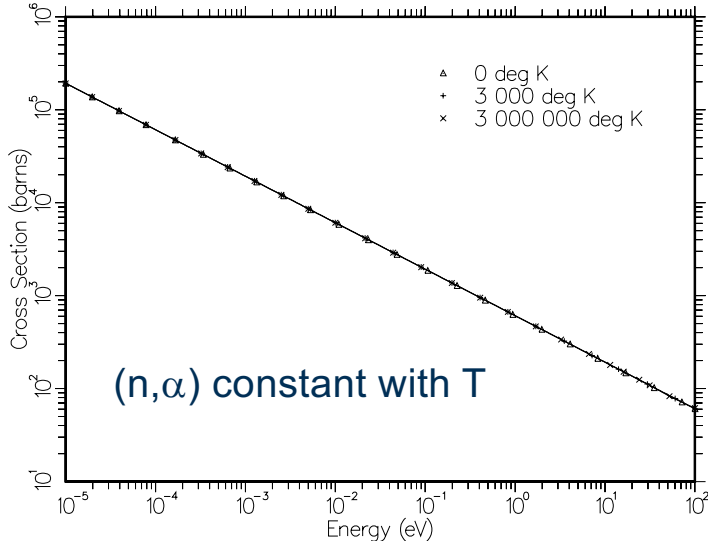
GND contacts: mattoon1@llnl.gov and beck6@llnl.gov

Derived nuclear data forms

Kerma, Damage Energy, Gas Production (Ni) Elemental



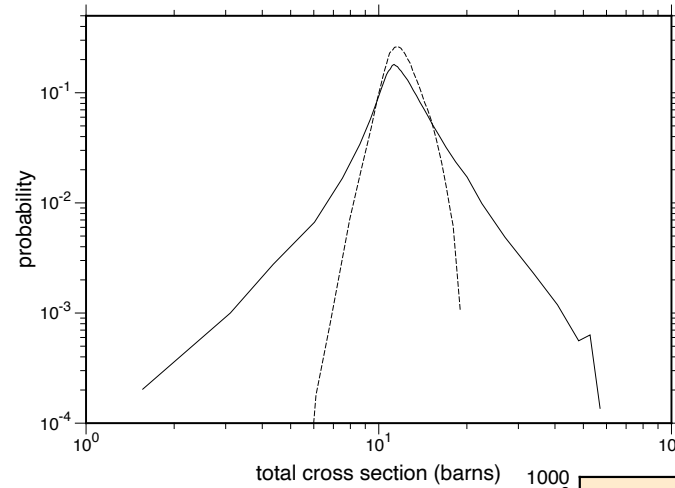
Pointwise ENDF, doppler broadening in the RR



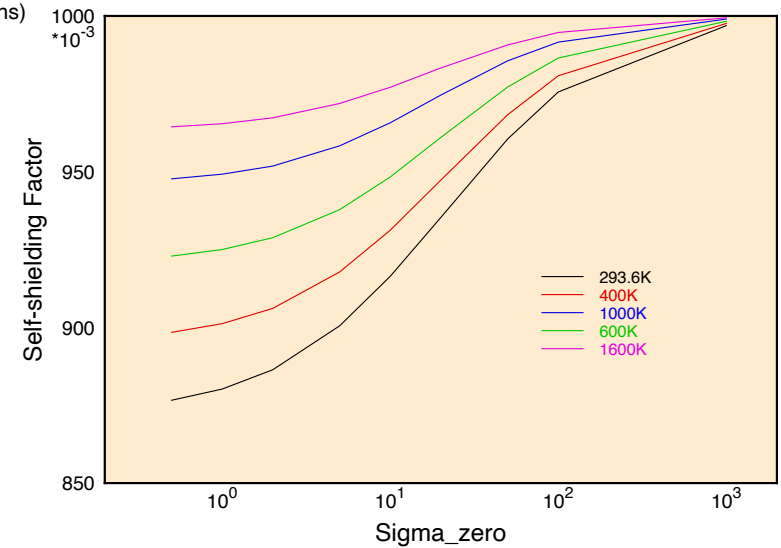
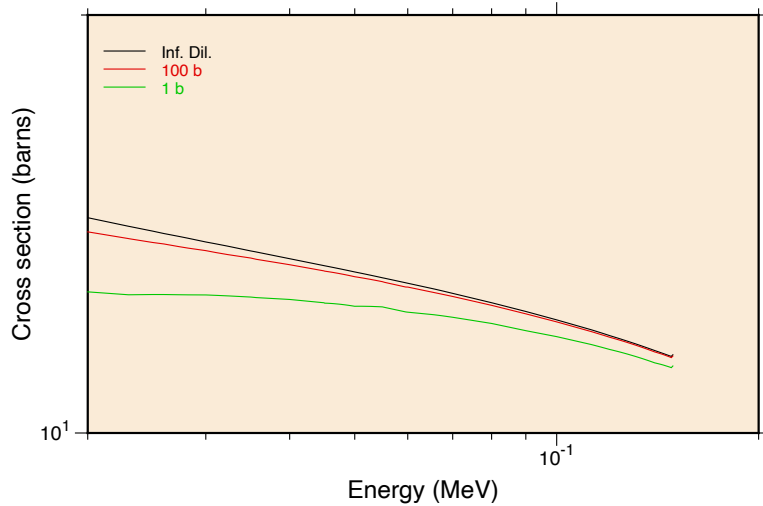
Hidden in the URR, PT's SSF

PDFs @ 20 keV,
dashed @ 140 keV

R. E. MacFarlane NJOY

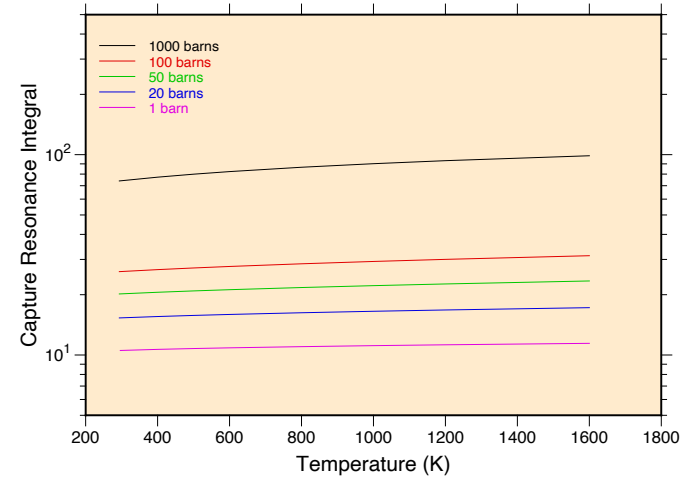
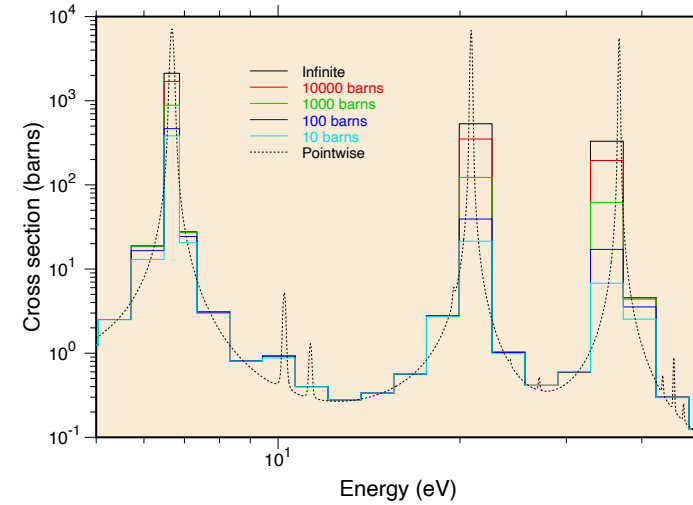
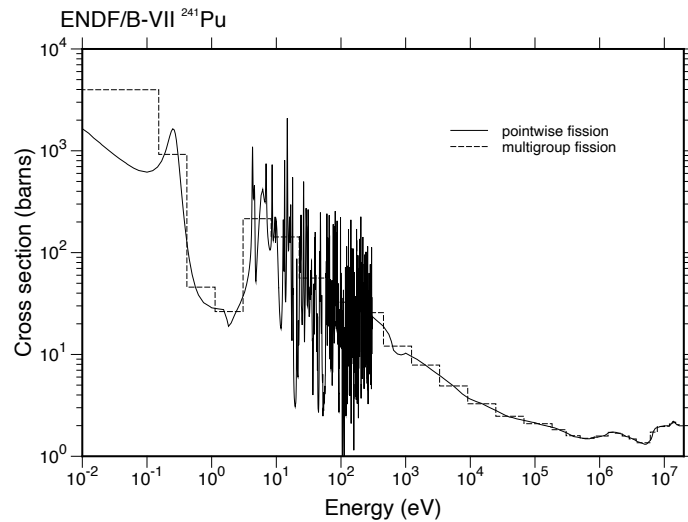
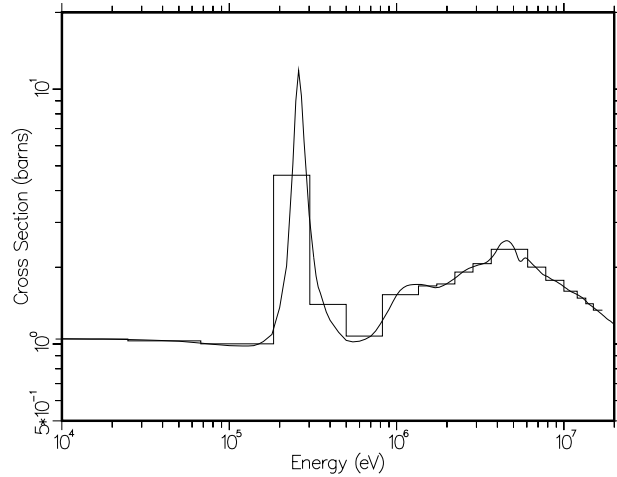


ENDF/B-VII U-238
UR total cross section



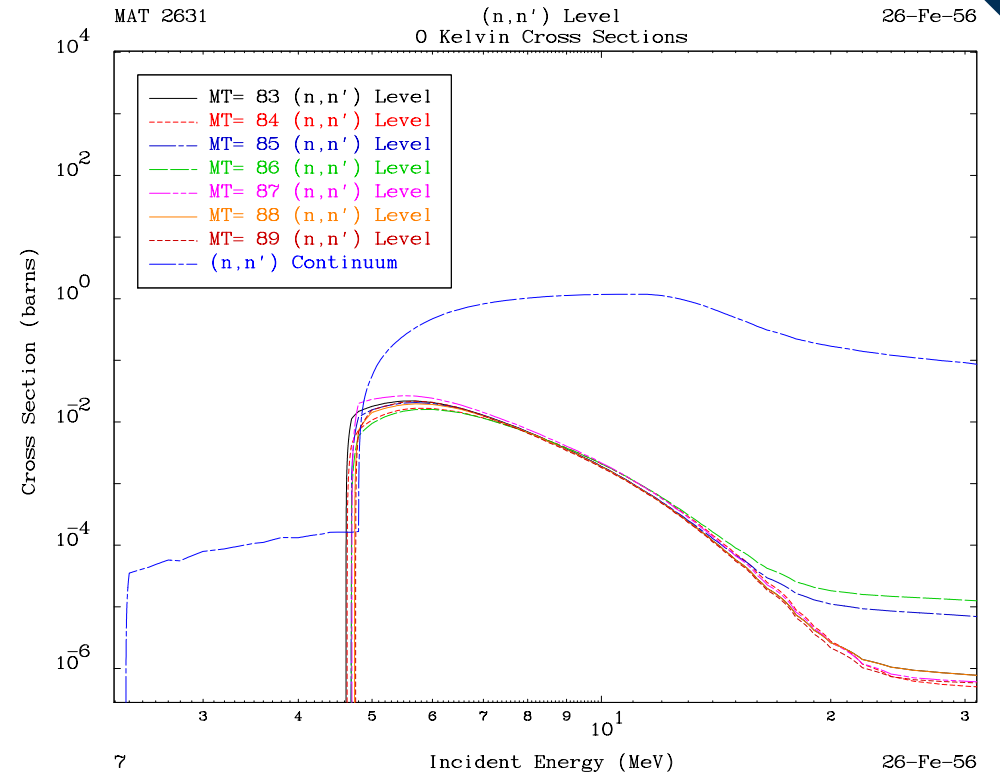
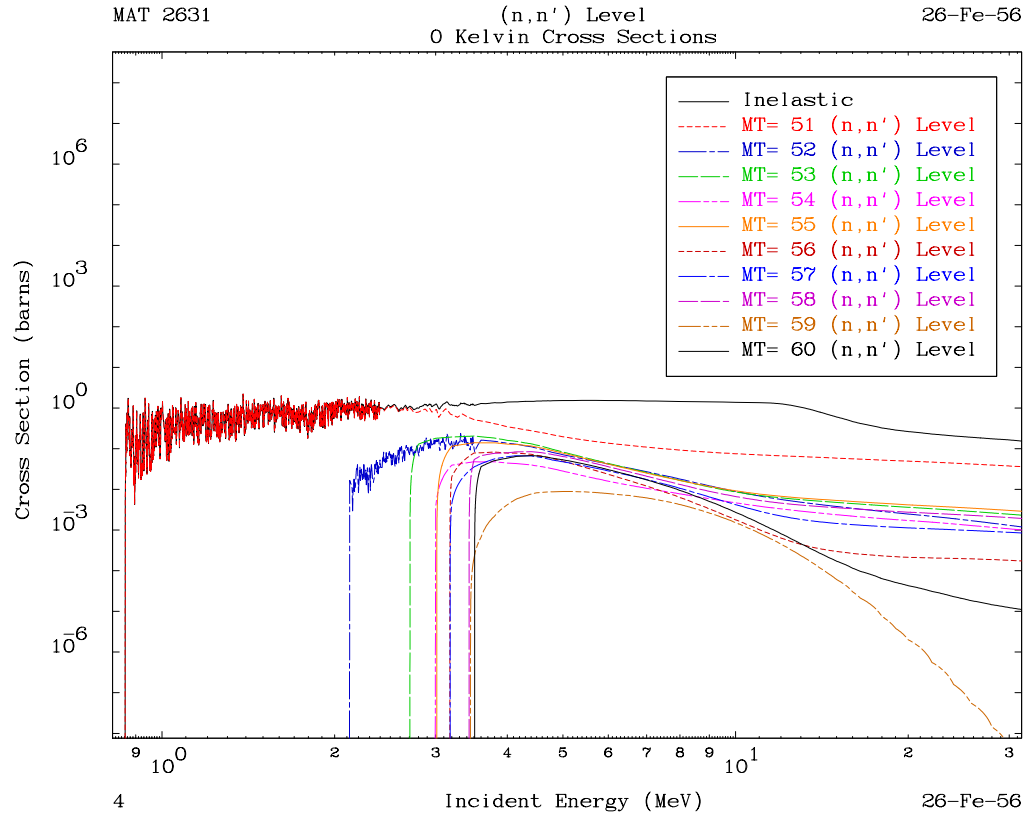
Groupwise ENDF and dilution, Bondarenko

SSF on U^{238} first 3 resonances



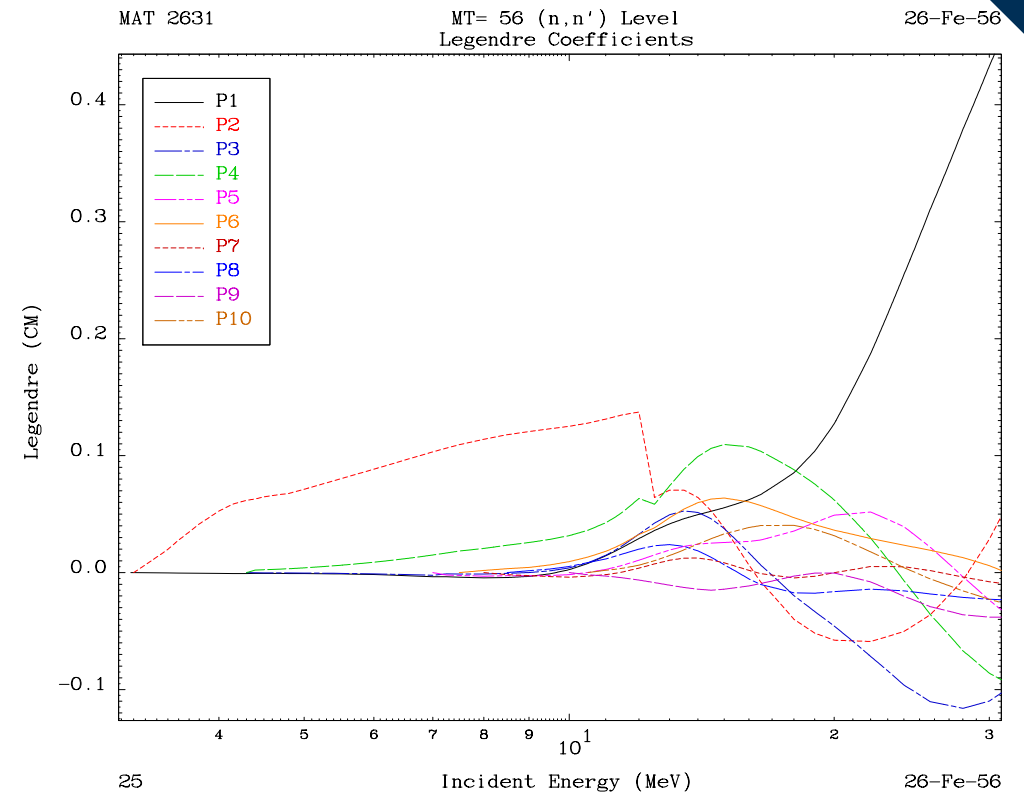
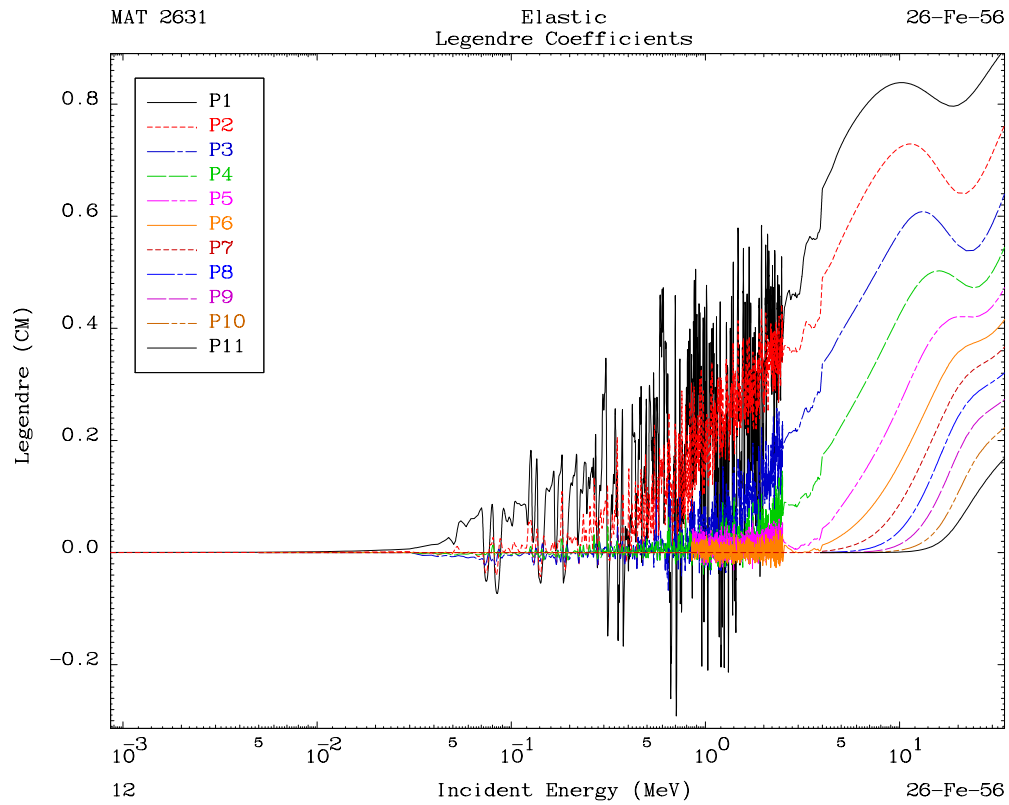
Slope with T = negative temperature coefficient

Partials and Legendre coefficients



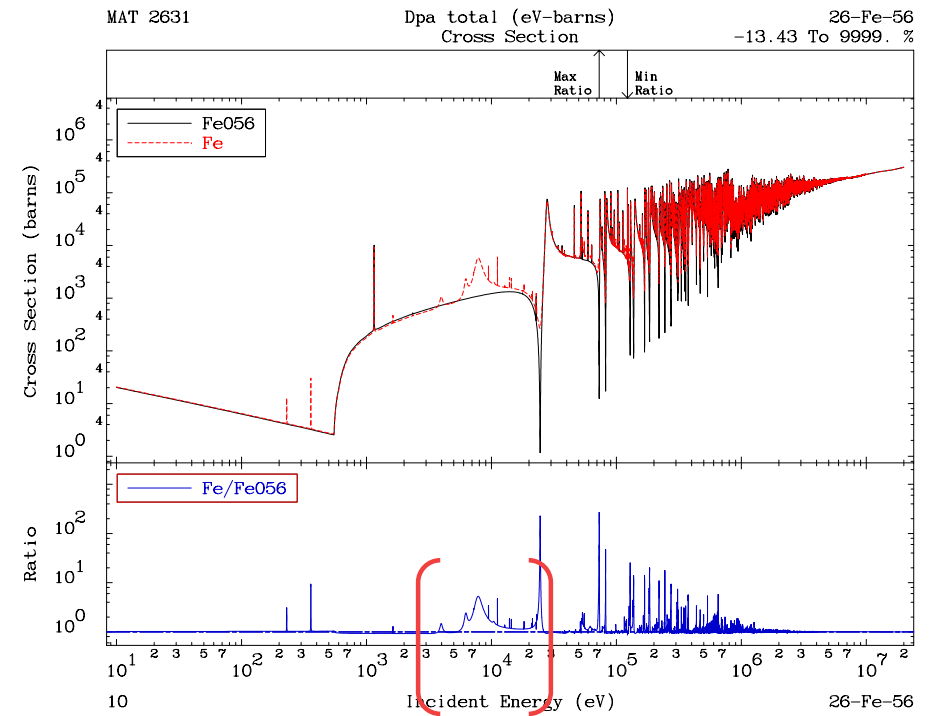
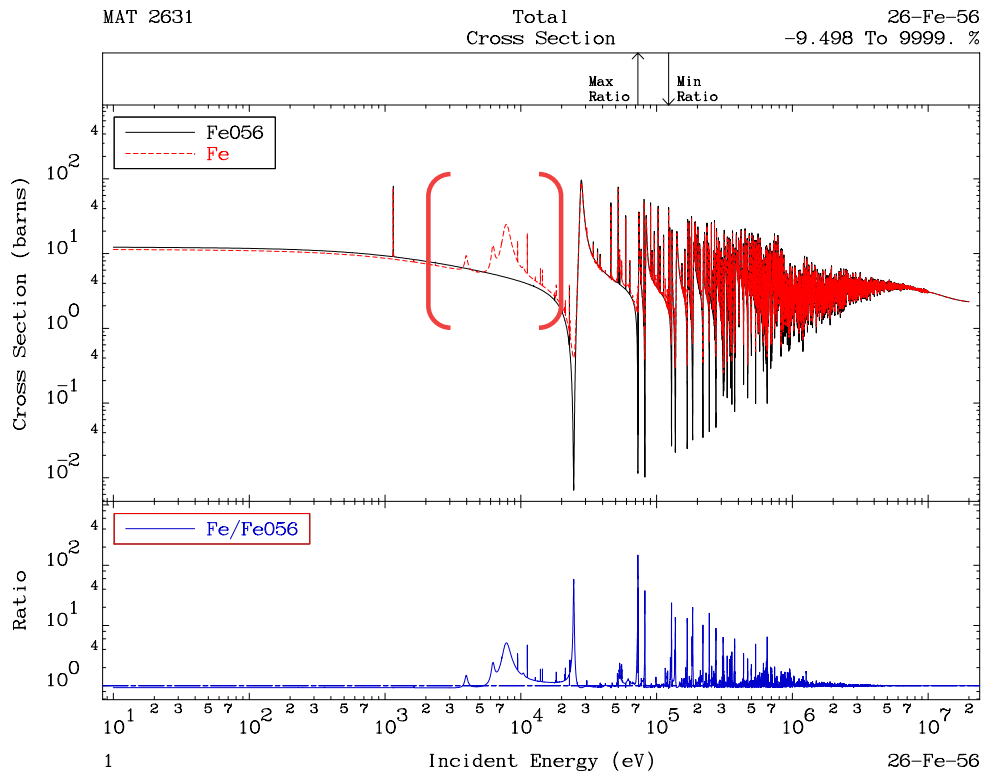
Fluctuations in MF-3
Not from resonance parameters in MF-2

Partials and Legendre coefficients

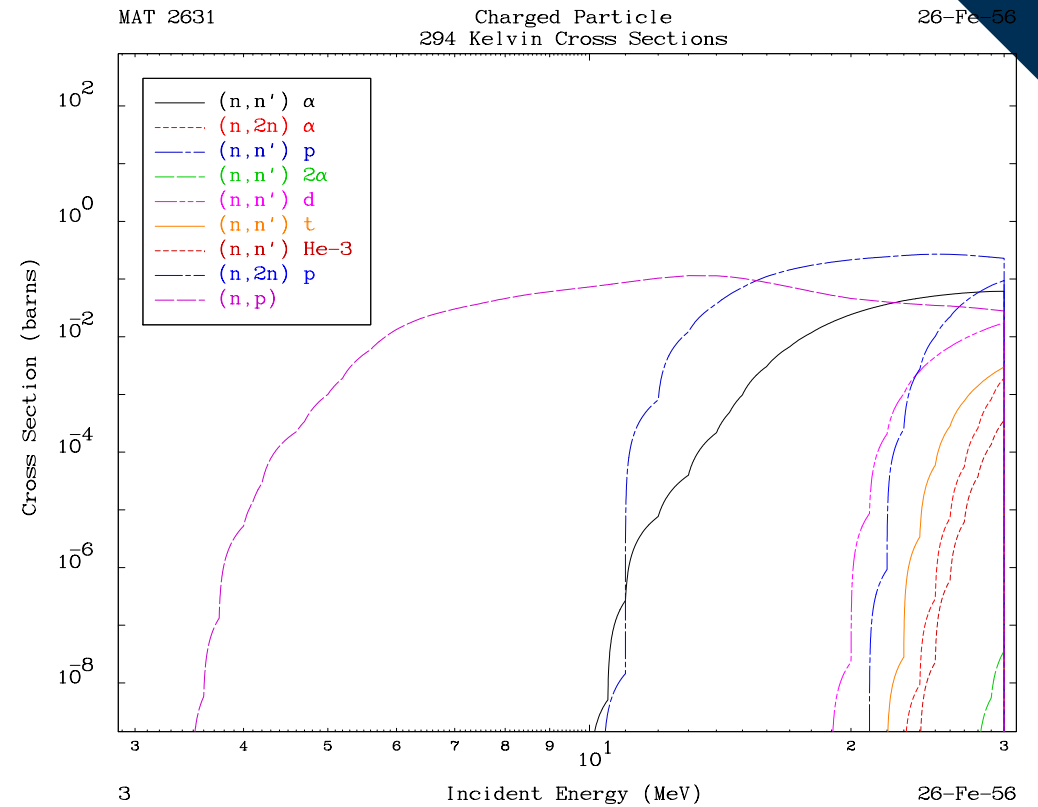
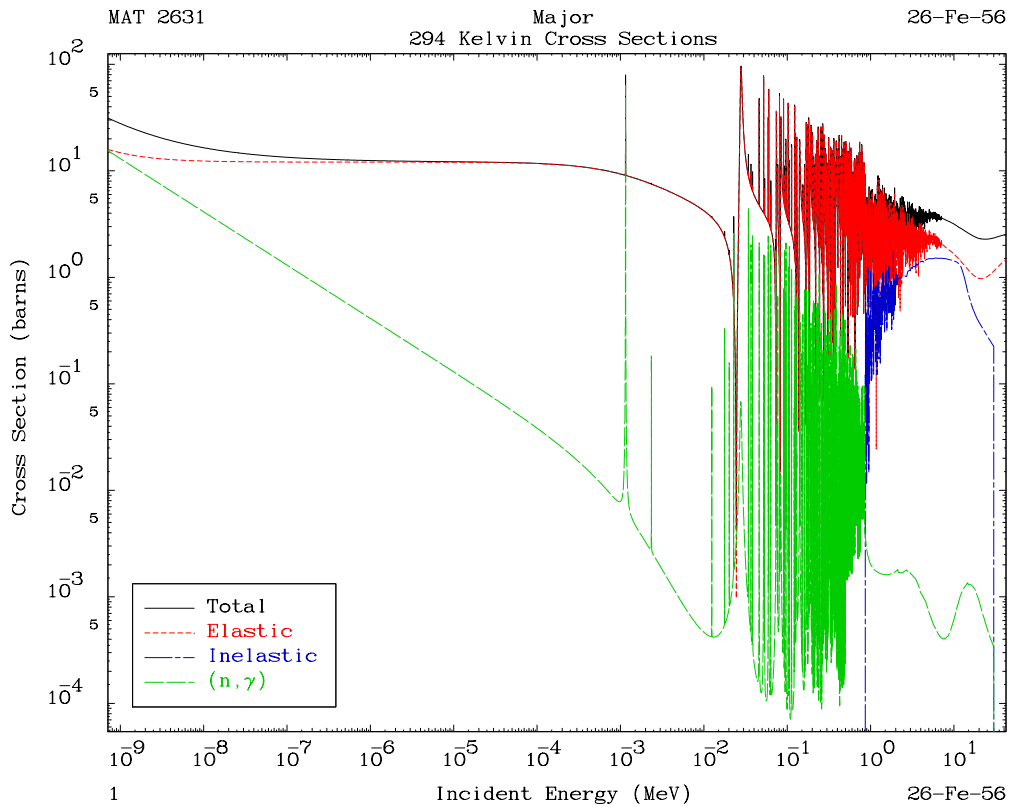


Total and Dpa: isotopic versus elemental

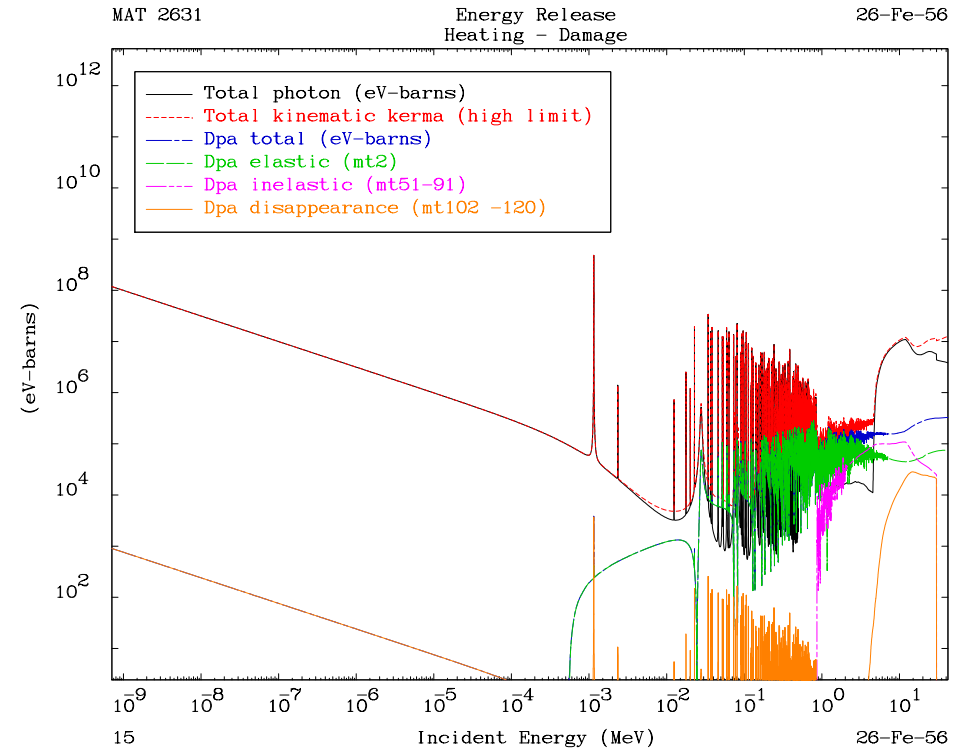
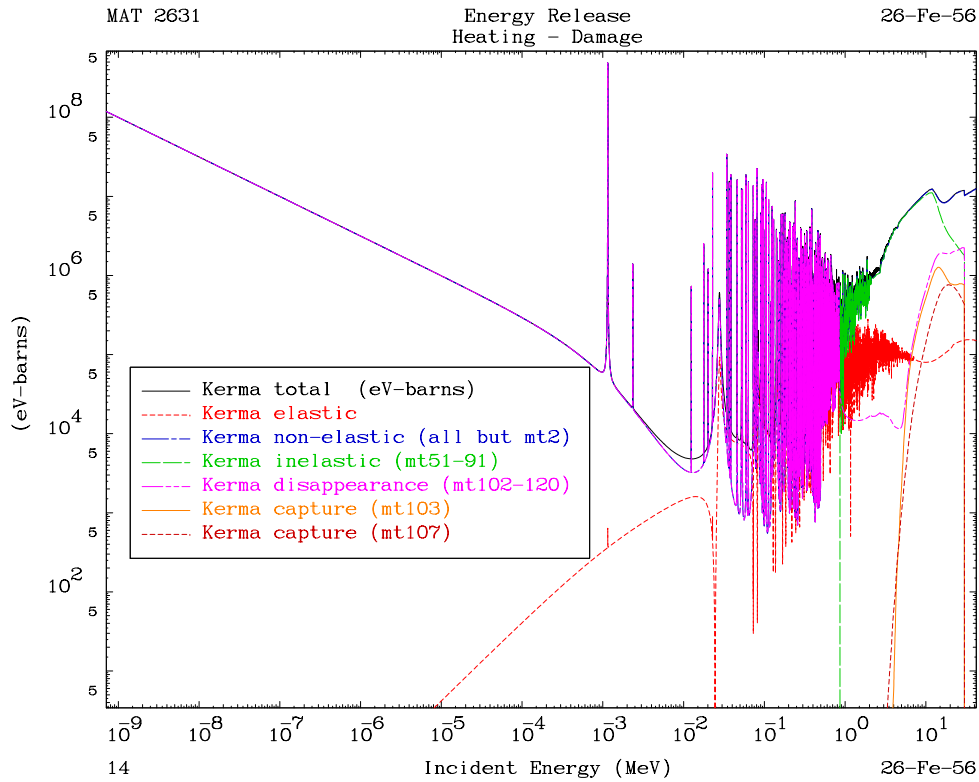
The energy range matters



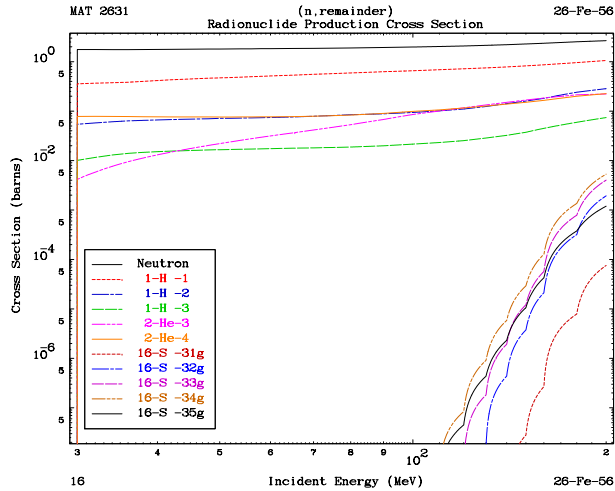
Major, charged particle, heating Kerma, DPA



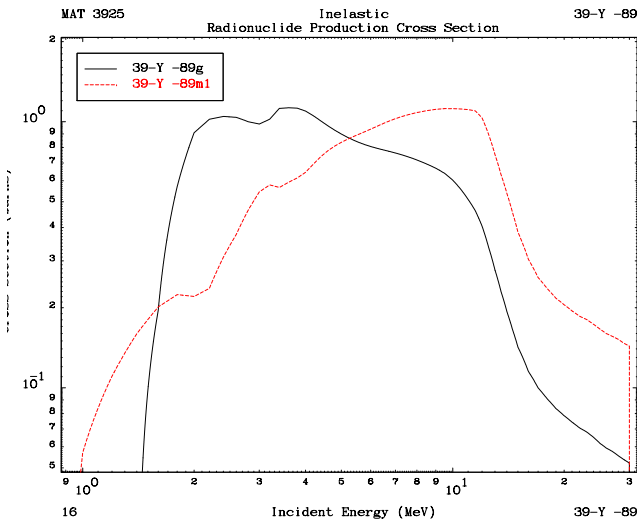
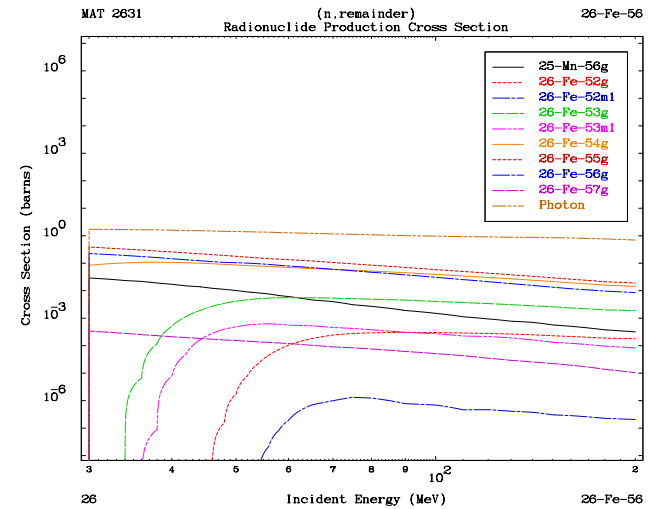
Major, charged particle, heating Kerma, DPA



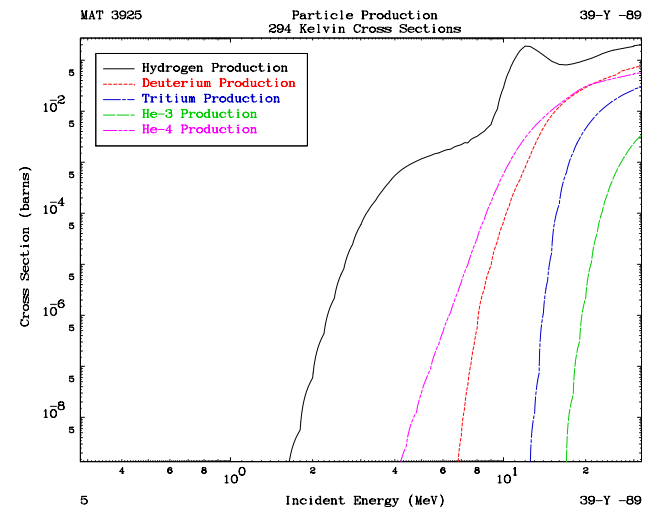
Implicit MF3-MT5*MF6 – isomer & gas production



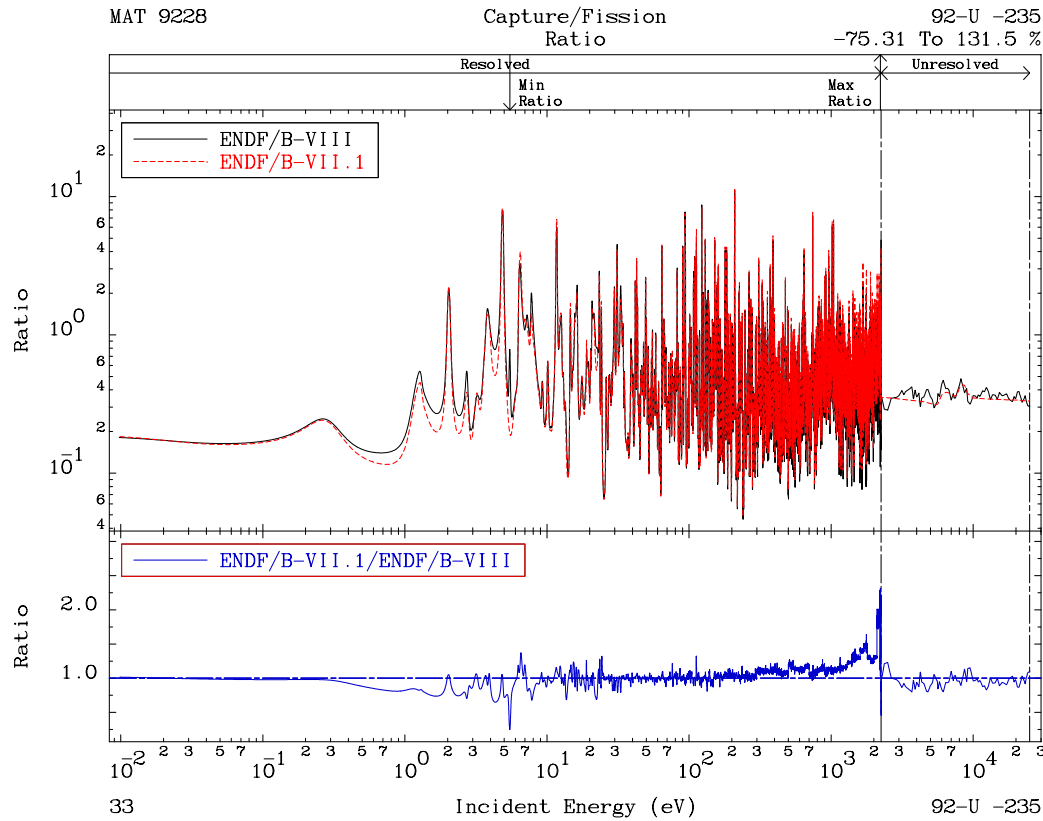
Hundreds of prod. yields
MF-8 dic.
MT-5*MF-6
using sixpack



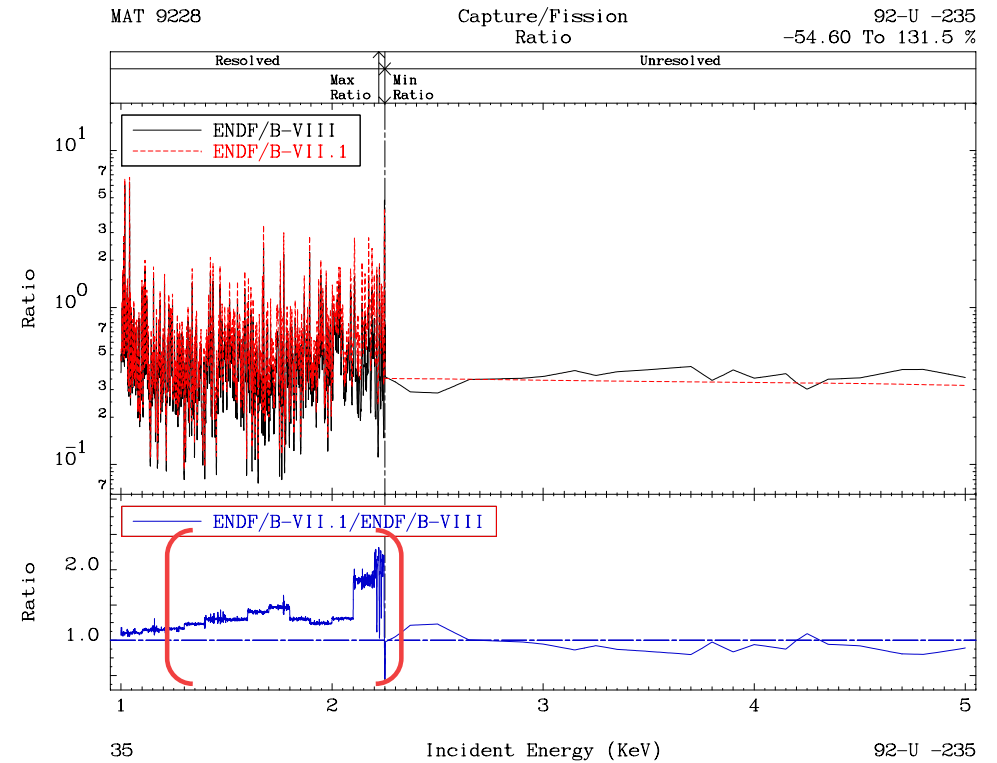
MF-10



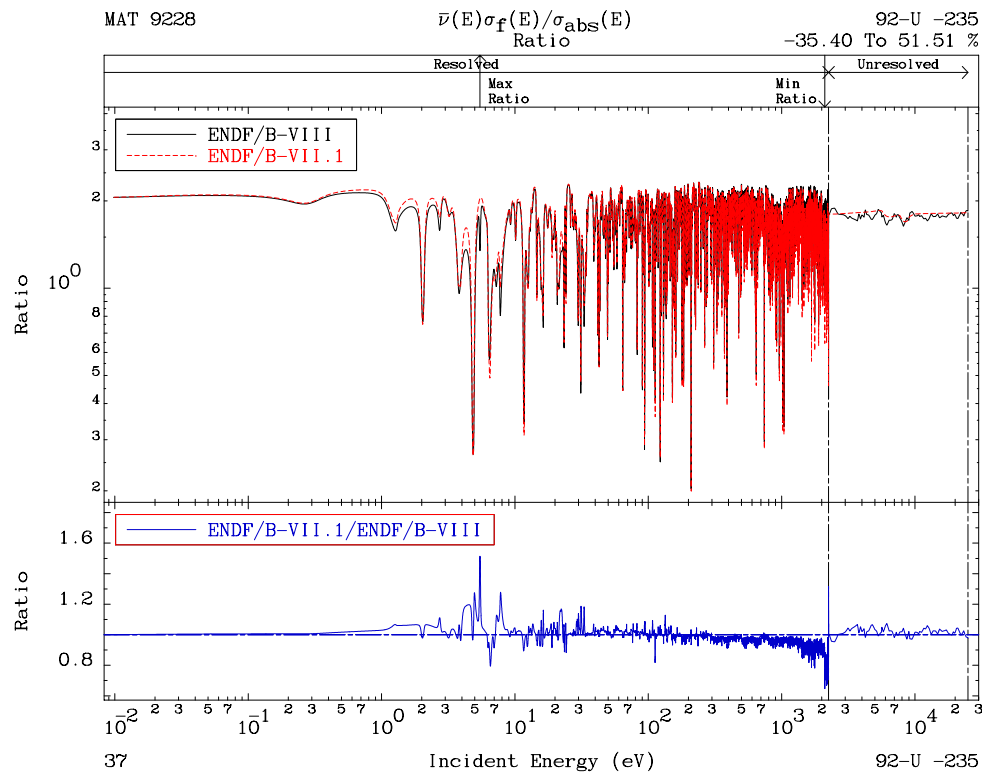
Derived quantities: capture/fission and alpha



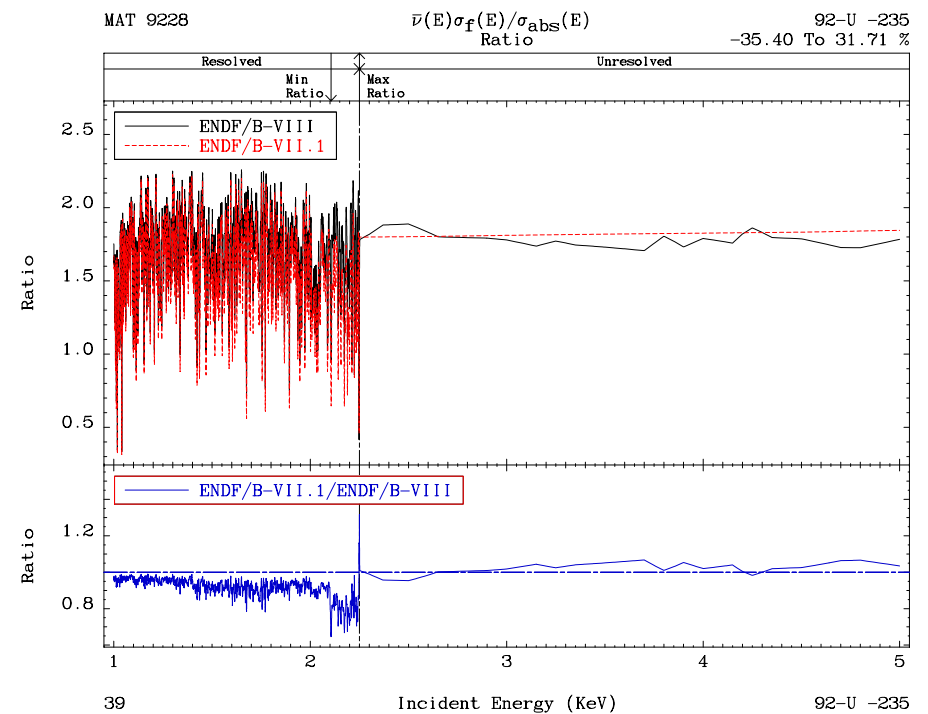
Steps show Keff tweaks !!



Derived quantities: capture/fission and alpha



Reactor parameter
Keff crits adjustment



Backend of data forms for data portal

Scripted, automatic, basic ENDF-6, GNDS-2.0 processing steps, parser and interpreter

Evaluated data forms need to be similar, identical to one used by an applications

Experimental data and Processed Evaluated data forms need to correspond

Check with original NDC https://www.ndc.jaea.go.jp/ENDF_Graph/



EXFOR statistics & quantity 10/2024

EXFOR dictionary and quantity codes would benefit from simplifying, decluttering, prioritizing

Expert groups, working parties can then be tasked to deliver a curated quantity serving prioritized process: e.g. DAE

Quality instead of quantity

Dictionary



Number of ENTRY	25274	experimental works
Number of SUBENT	168883	data tables (can contain data of more than one reaction)
Number of Datasets	186137	data tables of reactions
Number of Datapoints	20368415	total number of data points

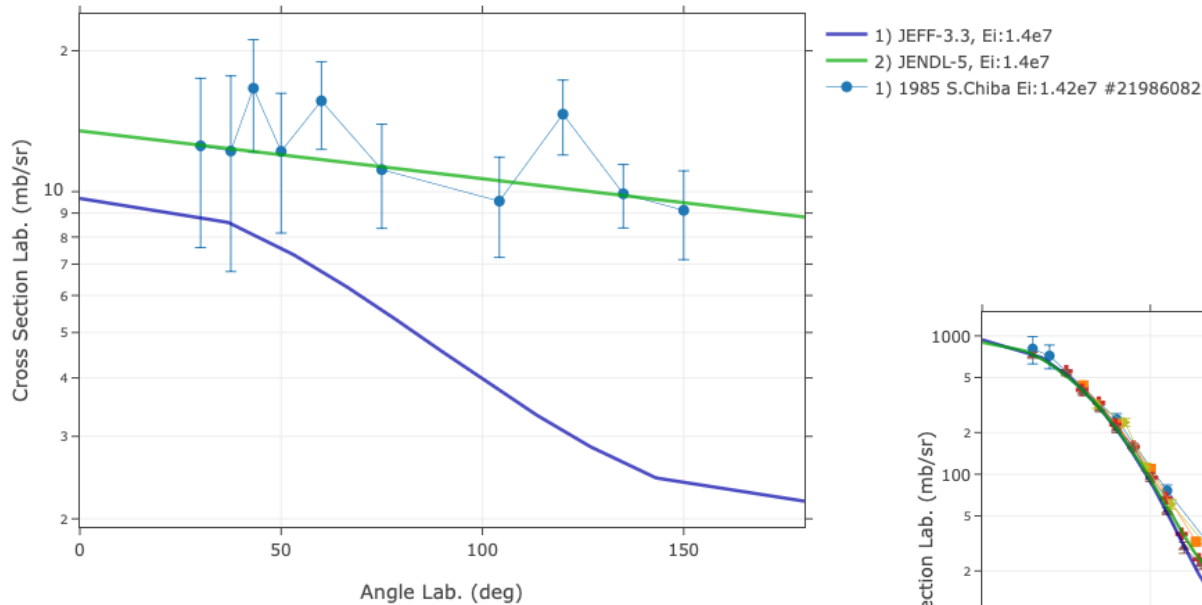
Percent: [Entries]/[Number of ENTRY], i.e. = [Entries]/25274
 Note. Σ [Percent] of a table below can be > 100% because one Entry (experimental work) usually contain many data tables with data of many types

EXFOR Quantity

#	Code	Quantity	Entries	Percent
1	CS	Cross section data	12910	51
2	DAP	Partial differential data with respect to angle	4923	19.4
3	DA	Differential data with respect to angle	4768	18.8
4	RP	Resonance parameters	2165	8.56
5	CSP	Partial cross section data	2122	8.39
6	FY	Fission product yields	1492	5.9
7	DAE	Differential data with respect to angle and energy	1230	4.86
8	POL	Polarization data	1201	4.75
9	NU	Fission neutron multiplicities	550	2.17
10	RI	Resonance integrals	501	1.98
11	SP	Gamma spectra	494	1.95
12	E	Kinetic energies	457	1.8
13	TT	Thick target yields	414	1.63
14	DE	Differential data with respect to energy	405	1.6
15	L	Scattering length	228	0.9
16	INT	Cross section integral over incident energy	221	0.87
17	ZAP	Most probable charge or mass	219	0.86
18	TTD	Differential thick target yields	164	0.64
19	MFQ	Differential fission neutron multiplicities	157	0.62
20	NQ	Nuclear quantities	123	0.48
21	RR	Reaction rates	121	0.47
22	MLT	Outgoing particle multiplicities	75	0.29
23	PY	Product yields	74	0.29
24	CST	Temperature dependent cross section data	65	0.25
25	TTP	Partial thick target yields	31	0.12
26	SQ	Special quantities	18	0.071
27	DEP	Partial differential data with respect to energy	16	0.063

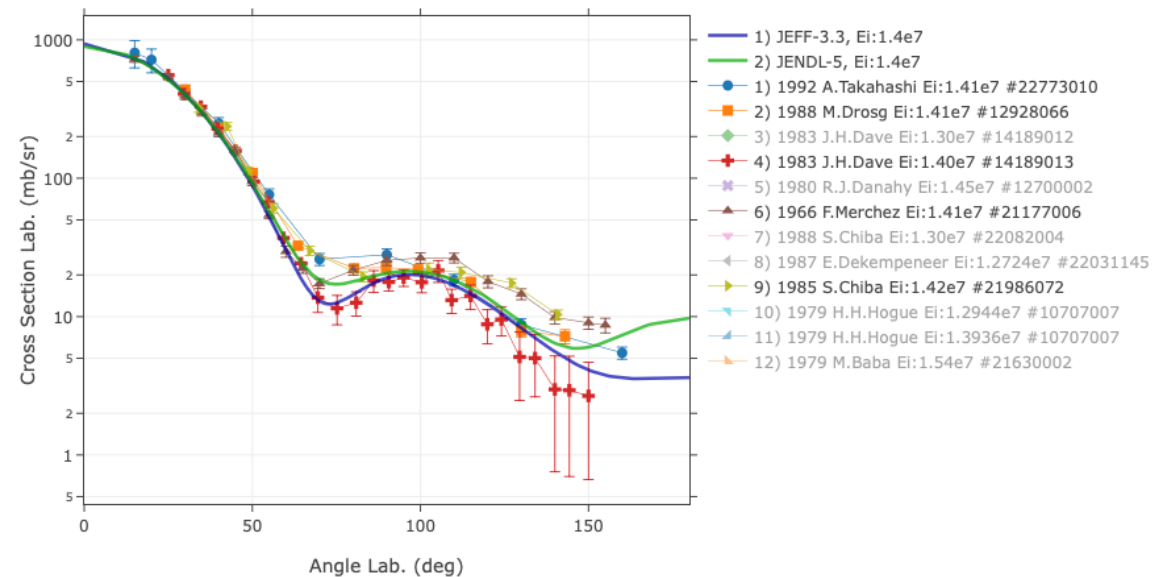
Processing steps - MF-4

Li-7(n,2n),da



PREPRO – LEGEND
only n-outgoing !

Li-7(n,el),da



EXFOR: DA, μ_{lab} ; evaluation μ_{cm}
0.96 to 1.0 CM cut-off angles
A = mass target/projectile

$$\mu_1 = \frac{(1+A\mu_c)}{\sqrt{A^2+2A\mu_c+1}}$$

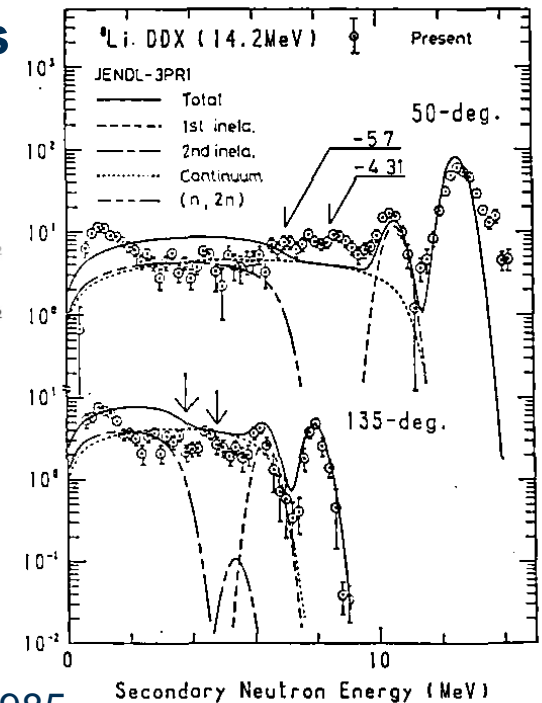
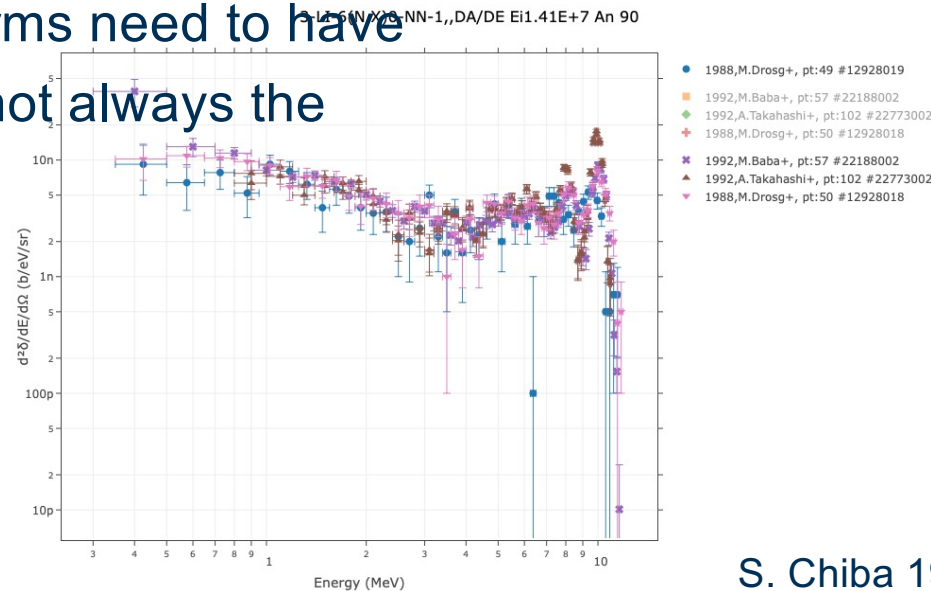
Processing steps - MF-6

The processing steps for evaluated DA/DE @ E_{in} from MF-6 entries to compare with experimental information mb/sr/MeV (lab) requires:

- Processing capabilities for all allowed format representations
- Accounting for all channels, levels: continuum, 1st, 2nd inelastic, (n,2n), ...
- Conversion to lab from cm co-ordinate for all observables

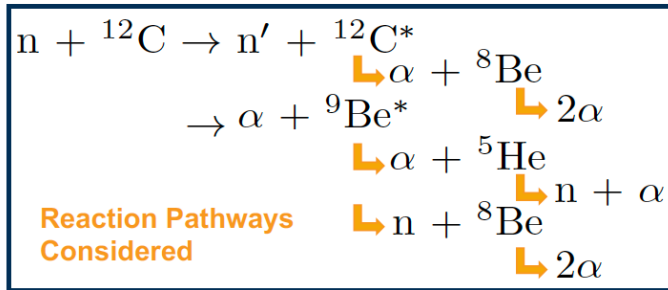
The experimental data forms need to have been properly compiled, not always the case, complex process

Works, not quite...

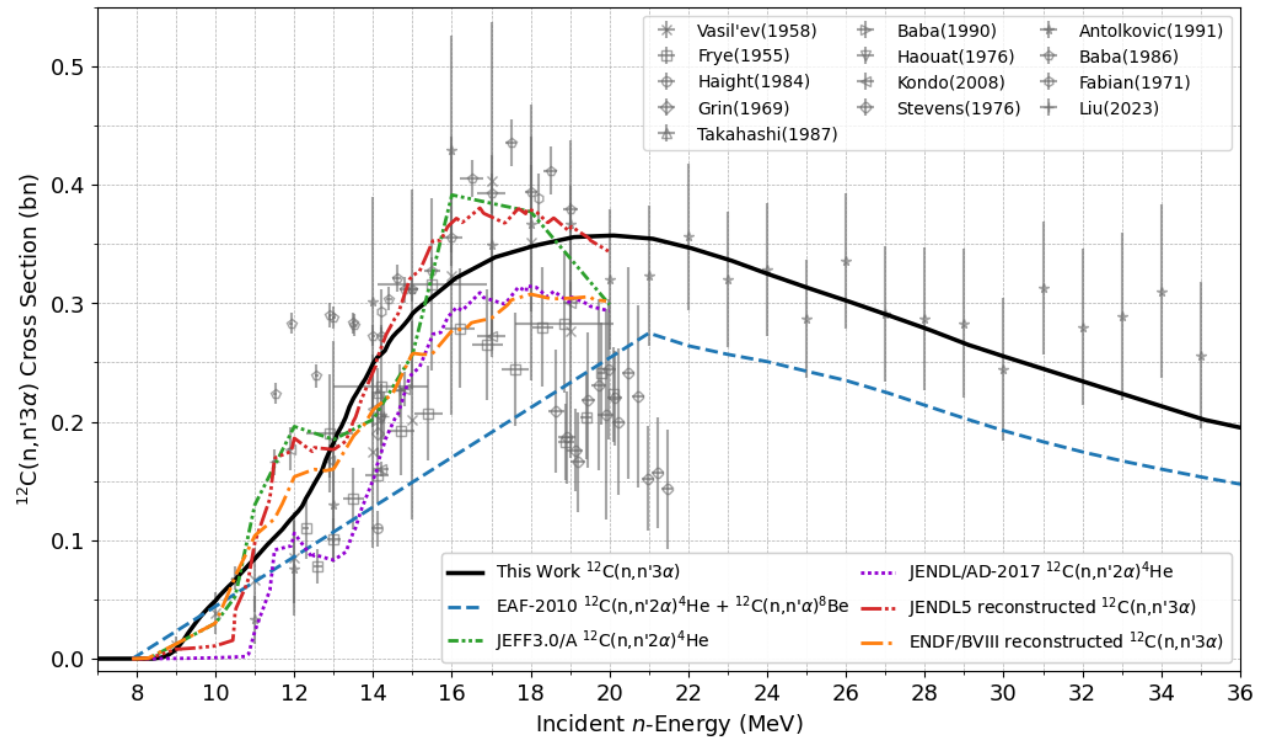
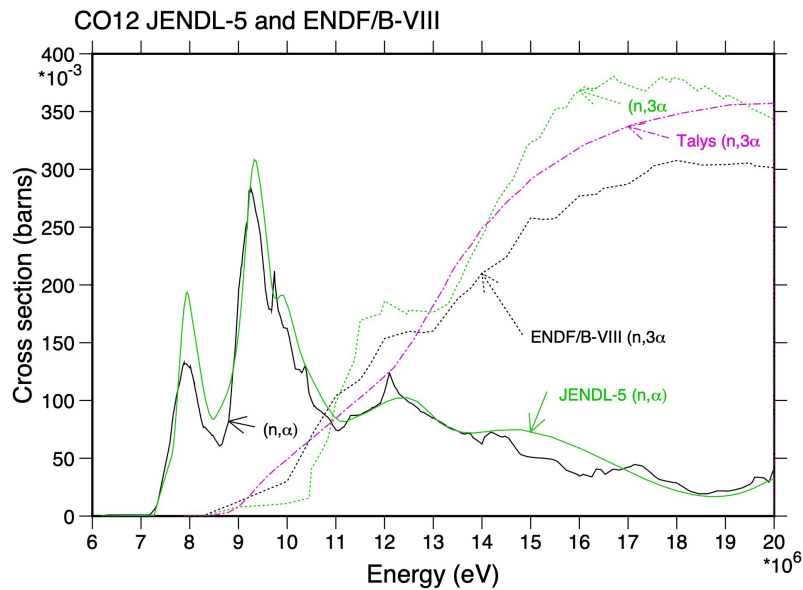


S. Chiba 1985

Processing steps, breakup, LR flags

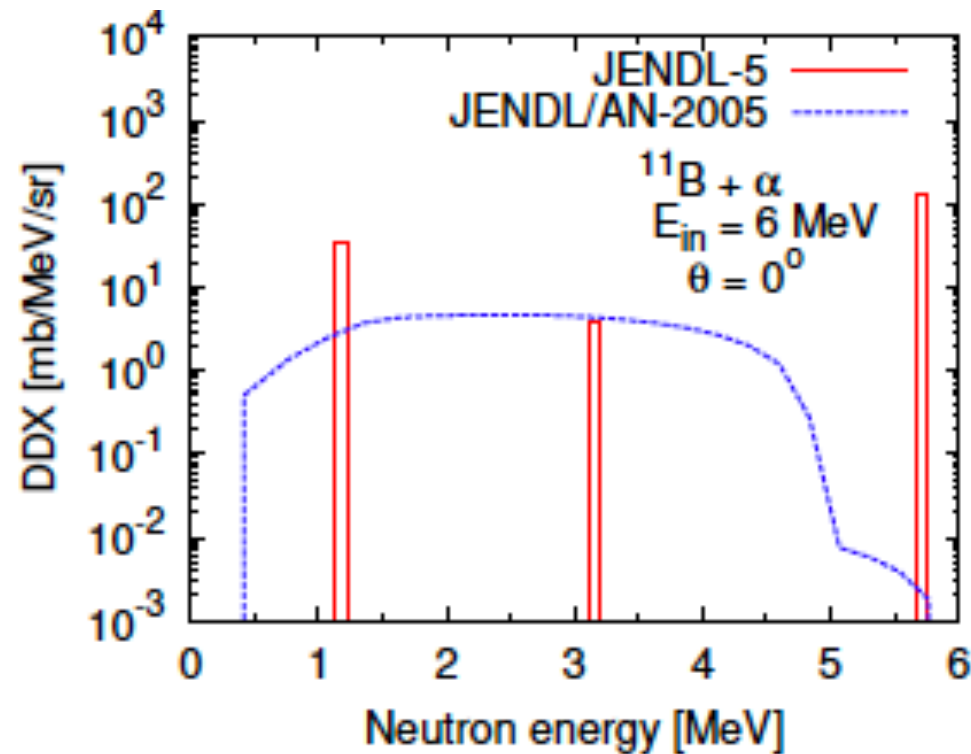


EXFOR measured quantity ??
 EXFOR ${}^{12}\text{C}(n,2\alpha+n){}^4\text{He}$ and ${}^{12}\text{C}(n,X){}^4\text{He}$
 MT=29



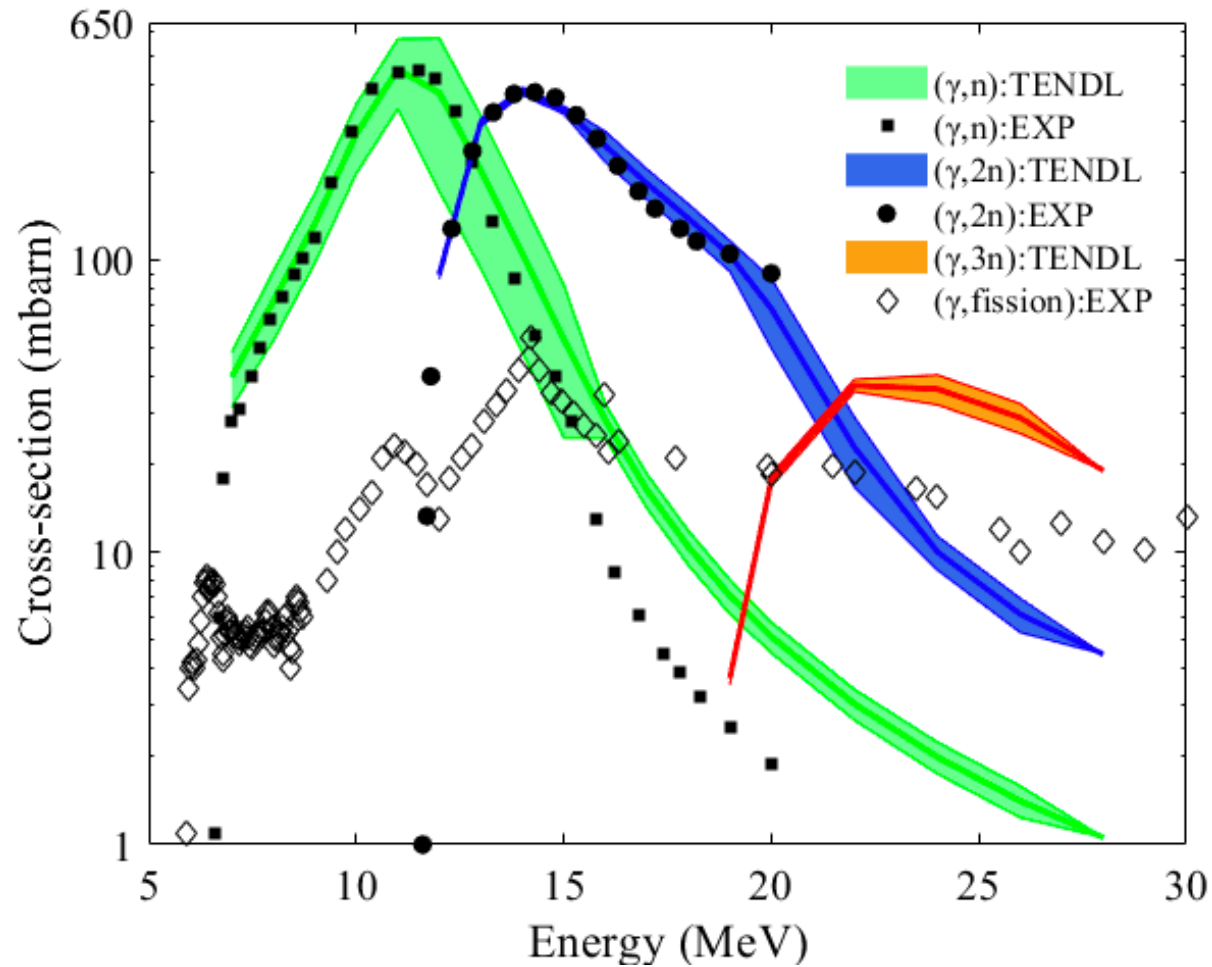
Challenges in interpretation – JENDL-5

- Discrete (α, n_0) , (α, n_1) and (α, n_2)
- Discrete peaks instead of continuous energy distribution



Better display - gamma induced

- Gamma on ^{232}Th



(γ, f) exists in TENDL but in MF=10

γ -induced explicit data forms

Conclusions

The processing steps, practices that can be envisaged for modern nuclear data portal forms benefit from:

- Relying on more than one processing systems, none are *complete*
- Target simple comparable experimental metrics
- Use open-source systems, preferably the same as the ones use for many other applications
- Rely on open-access steps, processes, practices
- Output simple, verifiable data forms, modern graphics
- Been externally audited, Verified and Validated V&V
- Associated with model code physics