IAEA
International Atomic Energy Agency
Atoms for Peace and Development

GNDS-2.0, FUDGE-6.2, TAGNDS-1.0 white paper

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White paper

- The purpose of the event is to assess the actual capabilities, successfully deployed methods, tools and protocols, and future needs in terms of nuclear model code outputs in the General Nuclear Data Structure and their processing into useful applications forms

- At the same time and in support of high-fidelity multi-physics simulation efforts, build a modern durable partnership between fundamental sciences and applications needs

Lexical semantics

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

} Structure Format

- Hybrid END File >>> from PREPRO, NJOY to JANIS, FISPACT-II,..
- Pointwise END File >> from NJOY, PREPRO, CALENDF…to many codes
- Groupwise END File >> from NJOY, PREPRO,CALENDF… to many codes
- ANISOtropy >> from TRIPOLI-4 to TRIPOLI-4
- A Compact Endf >> from ACER, FRENDY… to MCNP, SERPENT, OpenMC,…
- Probability tables >> from CALENDF, PURR… to FISPACT-II, MCNP, TRIPOLI,…
- PDF, CDF, TF >> from NJOY, PREPRO, FRENDY to MCNP, SERPENT, OpenMC, TART,…
- …..

- It is important to differentiate between:

  nuclear data form, format and formalism

Lexical semantics

- Hybrid END File
- Pointwise END File
- Groupwise END File
- Matrices, PKAs
- ANISO tropy
- A Compact Endf
- Probability Table
- Self-shielding factor
- PDF and CDF
- Tabulated Form
- ....

Nuclear data application forms
GNDS equivalent

Formalisms

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

Lexical semantics

- Pre-processing steps: convert the GNDS, ENDF-6 nuclear data into simple forms that can be interpreted, observed
- Processing steps: processes the GNDS, ENDF-6 nuclear data into complex forms useful for applications: particles transport, reactor analysis codes, high energy physics, activation-transmutation, radio protection, etc.
- Post-processing steps: verify either of the above steps

The lexical is ancient, as the 'tape' NJOY, PREPRO, CALENDF usually modular and sequential steps I/O uses. It belongs to the dawn of the nuclear-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

Modern processing trails

- Simple, open source, elementary numerical computing tool and recipe
- Jupyter notebook, verification & validation steps
- FUDGE support reading, viewing, modifying, assembling, checking and processing nuclear data in the GNDS format

- Caveats
  - Try not to push the numeric
  - Accuracy, precision (when measured) and error
  - 7 digits of precision !!
  - 0.1% reconstruction taken as 0.1% precision

ENDF-6 translation issues for TENDL-2021

- GIDI+ code requires a PoPs (GNDS Property of Particles) file that contains meta-stable aliases for all meta-stables in a data library
- Activation-transmutation-depletion applications library requires a unique definitions for meta-stables: target, residuals, decay structures
  - WARNING: multiple pids for "Br70_m1": {'Br70_e5', 'Br70_e6'}
  - WARNING: multiple energies for "Mn60_m1" using most common: [0.2719, 0.2718**5**, 0.2719**01**] MeV
- Deciphering the MF's landscapes
- Numeric, accuracy and reality

GNDS: Properties of Particles (PoPs) overview

- For some applications such as inertial confinement fusion, a micro-second half-life can be long enough to qualify a state as meta-stable, while for other applications much longer half-lives are sufficient

- A particle database allows users to define their own metaStable nodes for more flexible control over what nuclear states to consider as meta-stable

- https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html

Live chart of Nuclides levels

Livechart - Table of Nuclides -

www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html#lastnuc=Y88

List of updates Oct 2022 - Apr 2023 | **Mass chains** β and ec decays plotting | **Neutron Cross Sections** Resonance Integrals

Live Chart of Nuclides **nuclear structure and decay data**

Go to Nuclide: Y88 **Show Chart**

Ground State isomers | **Levels** | Gammas | Decay Radiation | Nuclear Moments | Neutron Capture | Fission Yields | Schema Plot

117 rows retrieved

Comments · **Click on a column header to open the guide** • **Uncertainty** for numeric values refers to the last digits of the value: **12.1 *23* means 12.1 ± 2.3** • **Data from ENSDF** ·

Definitions & Sources

CSV **Data API** **Evaluation**: E.A. McCutchan and A.A. Sonzogni **Publication cut-off**: 1-Nov-2013 **ENSDF insertion:** 2014-01 **Publication:** Nuclear Data Sheets 115, 135 (2014)

#	Nuclide	E_x [keV]	J^{π}_{order}	Band	$T_{1/2}$	$T_{1/2}$ [s]	Decay modes BR [%]	Isospin	μ [μ_N]	Q [b]	Additional data	Comments
1	$^{88}_{39}Y_{49}$	0.0	4-		106.626 d *21*	9212486 *1814*	ec β+ 100		-0.42 *1*	+0.16 *3*		
2	$^{88}_{39}Y_{49}$	231.927 *25*	5-		0.8 ns *1*	800E-12 *1*						
3	$^{88}_{39}Y_{49}$	392.86 *9*	1+		0.301 ms *3*	0.000301 *3*	IT 100					
4	$^{88}_{39}Y_{49}$	674.55 *4*	8+		13.98 ms *17*	0.01398 *17*	IT 100		+4.88 *3*	+0.06 *6*		
5	$^{88}_{39}Y_{49}$	703.83 ? *14*	(7)+									
6	$^{88}_{39}Y_{49}$	706.79 *13*	2-		> 10 ps	10E-12						
7	$^{88}_{39}Y_{49}$	707.4 *4*	1+,2+,3+									
8	$^{88}_{39}Y_{49}$	715.12 *13*	(6)+									
9	$^{88}_{39}Y_{49}$	766.22 *16*	(0)+		2.4 ps *+13-6*	2.4E-12 *10*						
10	$^{88}_{39}Y_{49}$	843.04 *12*	(5)+		1.8 ps *+9-3*	1.8E-12 *6*						
11	$^{88}_{39}Y_{49}$	984.66 *13*	(4)+		0.82 ps *8*	820E-15 *8*						
12	$^{88}_{39}Y_{49}$	1088.21 *10*	(4,5,6)-									

Processing trails: example with three interlinked codes

ENDF file

- **NJOY-2016**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - purr
    - acer
    - groupr

pendf

- **PREPRO-2023**
  - linear
  - recent
  - sigma1
  - sixpack
  - activate
  - merger
  - dictin
  - groupie
  - legend

pendf

- **CALENDF-2010**
  - calendf
  - regroutp
  - condentp
  - lecritp
  - ….

PT table

ACE

HDF5

Spectra-PKA

CASMO

WIMS

ERANOS

….

Applications forms

FISPACT-II

Single script for an entire library

Done over the week-end

TENDL-2021 & JEFF-4T2 form issues

- **FUDGE** is a nuclear data package built around Python that supports reading, viewing, modifying, writing and processing nuclear data in the **GNDS** format
- **FUDGE-6.2.0** release with support for GNDS-2.0 specification https://github.com/LLNL/fudge

```
#!/bin/csh
#
set isma = (`cat ../iso-mat.jeff4-tr`)
#
set nbriso = $#isma
@ nbriso/=2
#
set count = 1
set c1 = 1
set c2 = 2
#
while ($count <= $nbriso)
    echo 'Fudge  JEFF-4.0T2' $isma[$c1] $isma[$c2]
#
    ln -s ../Orig/$isma[$c1]  .
#
echo 'running fudge'
   endf2gnds.py $isma[$c1] -v --continuumSpectraFix >& output
   echo 'saving output, pendf,  files'
   mv $isma[$c1].gnds-covar.xml gnds/.
   mv $isma[$c1].gnds.xml gnds/.
   mv output inout/out$isma[$c1]
#
    rm $isma[$c1]
#
    @ count++
    @ c1+=2
    @ c2+=2
end
```

endf2gnds translation

gnds.xml

gnds-covar

TENDL-2021 GNDS/Xml ✓

630 Neutron induced, **s30**

282 Proton, Deuteron, Alpha and Gamma induced

https://tendl.web.psi.ch/tendl_2021/tar.html

JEFF-4T2 GNDS/Xml

54/562 failed translation

Usual ~5-10% rate

Succesfull translation output information

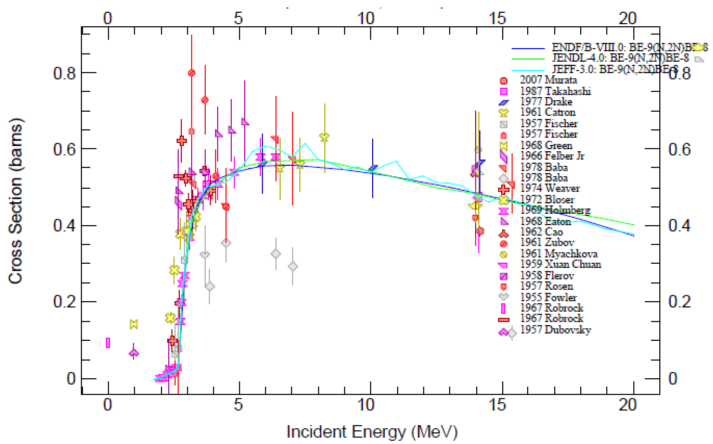
```
 2 [3, 4, 33] : MF=4, LTT = 3
      51 [3, 4, 12, 14, 33] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
      52 [3, 4, 12, 14, 33] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
      53 [3, 4, 12, 14, 33] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
      54 [3, 4, 12, 14, 33] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
      55 [3, 4, 12, 14] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
      56 [3, 4, 12, 14] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
      57 [3, 4, 12, 14] : MF=4, LTT = 1 : MF=12 LO=2 : ZAP=0 : MF=14
        WARNING: sum of gamma BR's for MT=57 MF=12 is 0.999999 != 1.0
*****
 103 [3, 6, 33] : MF=6 : ZAP=1001, LAW=1, LANG=2 : ZAP=23051, LAW=1, LANG=1 :
ZAP=0, LAW=1, LANG=1
 5 [3, 6, 8] : MF=6 : ZAP=1, LAW=1, LANG=2 : ZAP=1001, LAW=1, LANG=2 :
ZAP=1002, LAW=1, LANG=2 : ZAP=1003,…….
*****
 Reading resonances (MF=2 MT=151)
    Reading covariances (MFs 33,40)
    Reconstructing resonances
From 0.000010 to 9505.527000 eV, reconstructing using Multi-level Breit-Wigner
        WARNING: sum of gamma BR's for MT=57 MF=12 is 0.999999 != 1.0
        WARNING: sum of gamma BR's for MT=65 MF=12 is 1.00000101 != 1.0
6301 points were added (for total of 16325) to achieve tolerance of 0.1%
*****
WARNING: MT58 MF12 level energy 1039999.0 differs from MF3 value 1040000.0.
Setting to MF12 value.
WARNING: MF32 resonance parameters differ for 28 resonances
WARNING: MF=4 data for non-neutron product: MTs = [600, 601,…
Exception: Discrete two-body must be in the center-of-mass frame: LCT = 3 MT = 601
```

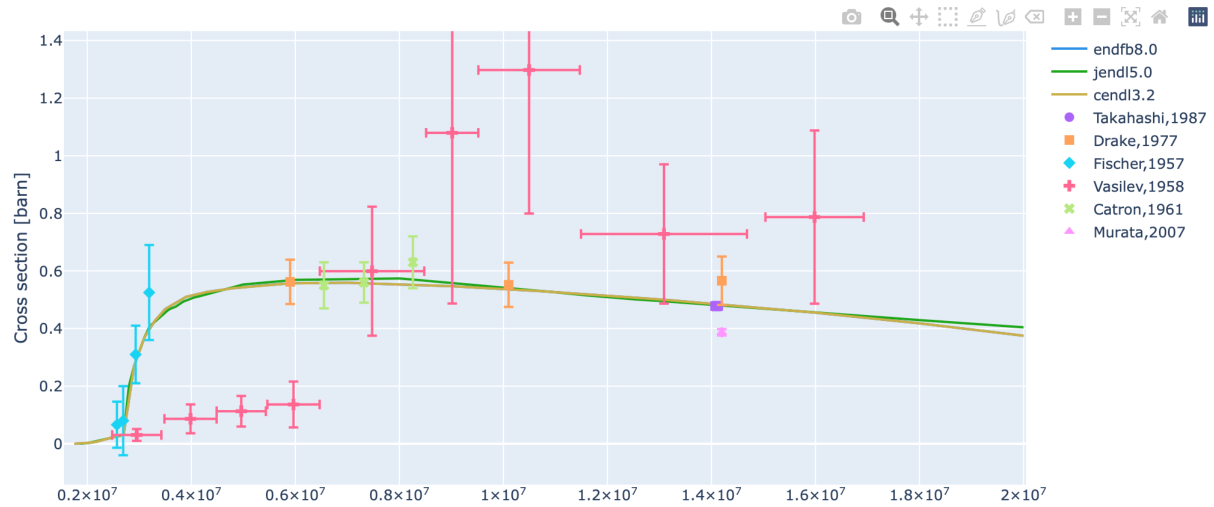
TENDL-2021 & JEFF-4T2 form issues

- MF8, MF=9, MF10, MF40 energy level consistancy issues within a file:
  - Ag106m,Ag107, Ag109, Co62m, Cr050, Cr053, Cr054, Eh152m, Eu154, Ho166m, Lu176, Nb094m, Pu237, Pu239, Ta180m, Tc099, Te127m, Te132, U235, W183, Xe135
- TALYS/TEFAL glitch when JEFF-4T2 = TENDL-2021 e.g. Pu237. ELFS U235m 7.600000+1 and not -2.147484+9 !!
- JEFF-4T2 = TENDL-2021 Pm148m Unique MT5 radioactive product Xe133_e1 not found in product list
- JEFF-4T2 = TENDL-2021 U239, U240 energy boundaries out of order in MF31 MT452
- …

ENDF-6 legacy, ambiguous definitions

- Be009 issue: 'item with label = "2n + 2He4" already present in suite'; reaction or decay ?? Back to the definition of event and its timing: discrete, isomeric states, break-up, decay
- n + ^{9}Be ➔ ^{8}Be (~10^{-17}s - Decay $\alpha + \alpha$) + 2n (RTYP 44)
- ^{8}Li β^{-} ➔ ^{8}Be ➔ 2α https://www-nds.iaea.org/dataexplorer





Mode of decay but without decay as Be has a half life of the order of compound-nucleus formation times !! Decay file exists !!

TENDL-2021 & JEFF-4T2 issues

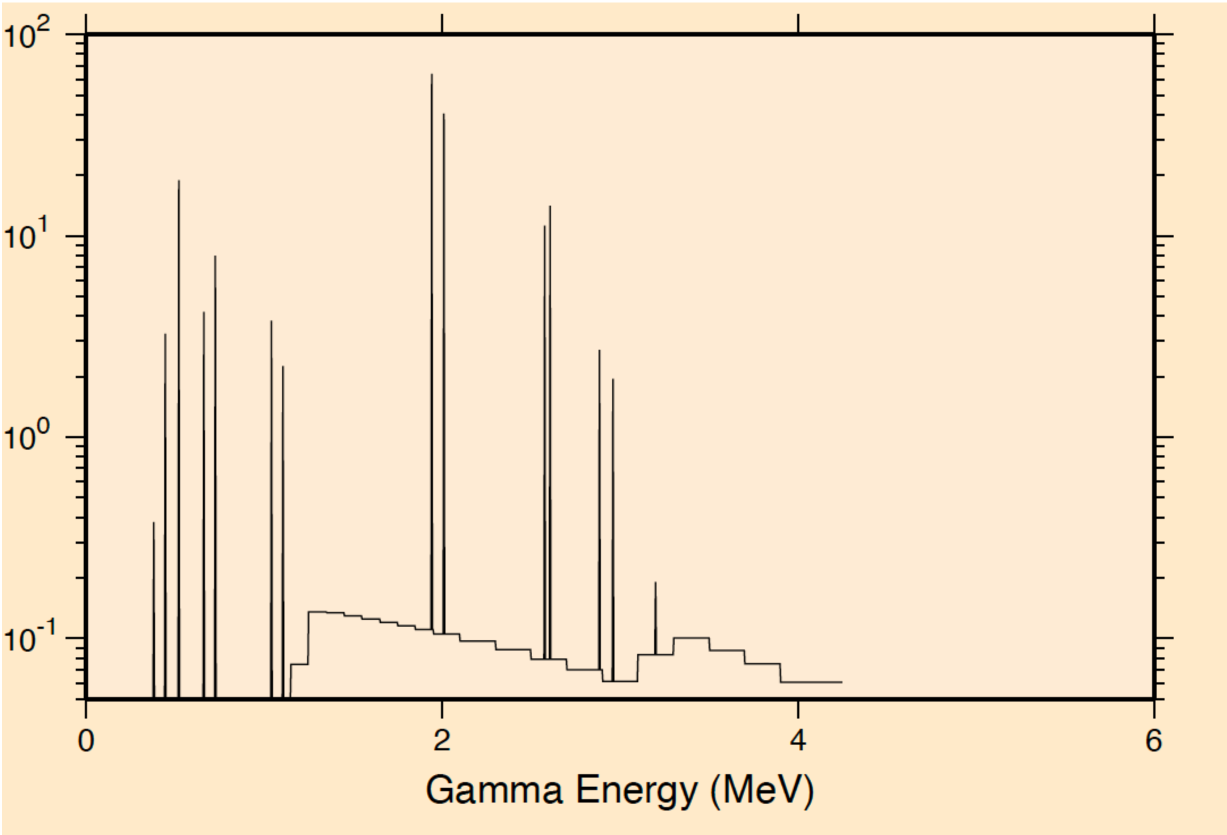
- B010 issue: MT700 lumped sum covariance is present, but no reactions are included in the sum!

The thorough ENDF6 to GNDS translation done or attempted by FUDGE probe the nuclear data physics, form and format like no other checking code ever did !!

ENDF-6, GNDS evaluated forms true coexistence

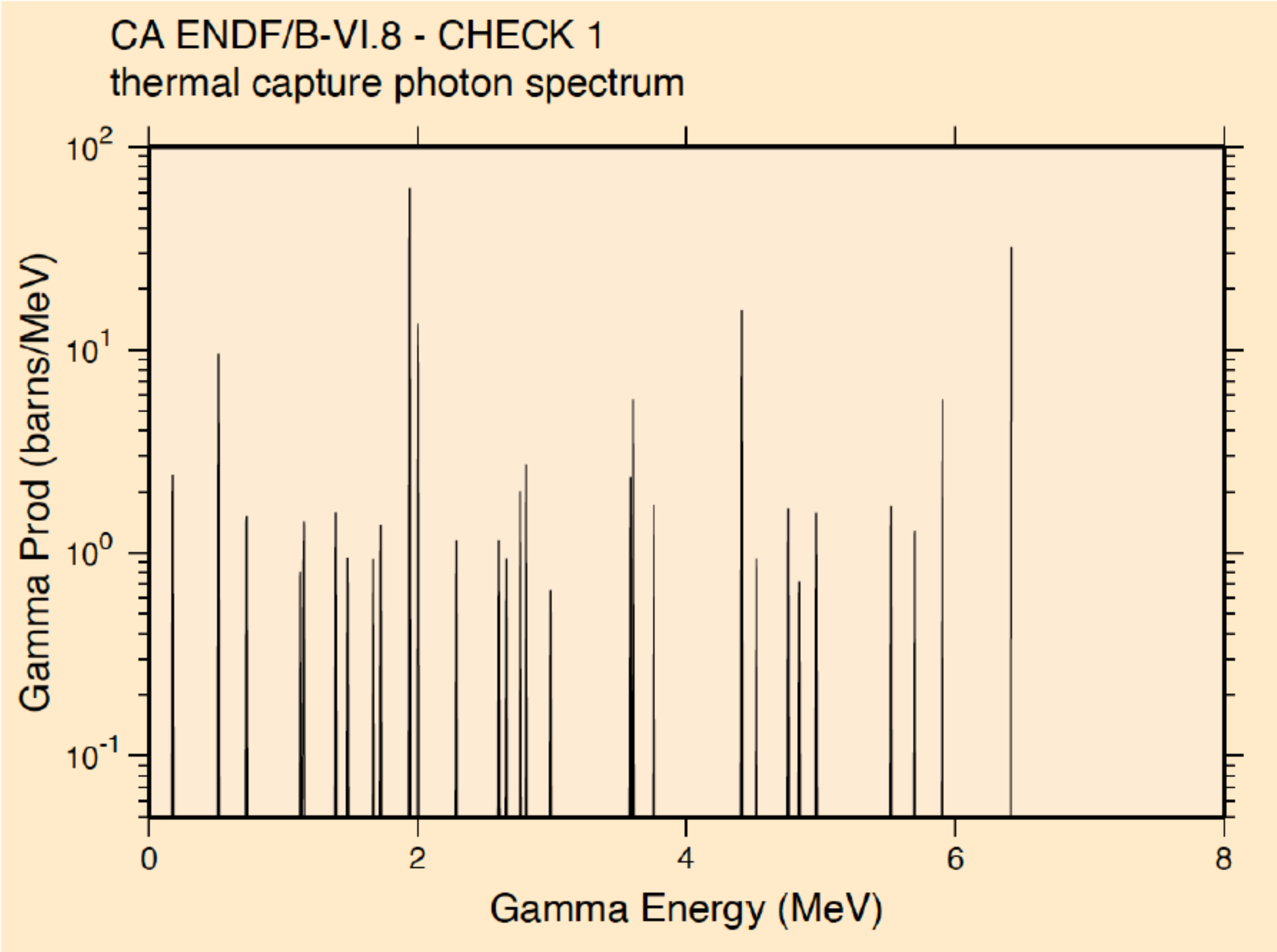
Challenges

- Enhanced completeness in the evaluation
- Better physics to answers all foreseeable applications instead of only THE one
- Detailed production of all γ-rays, emitted charge particles and residual nucleus states for every accounted events



Challenges

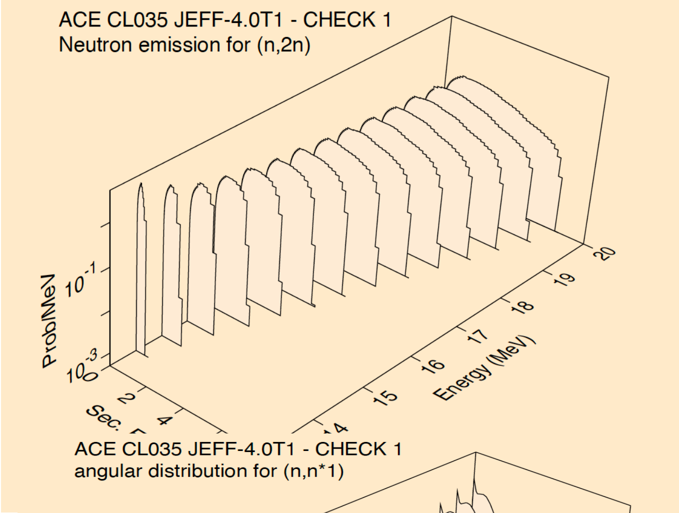
- Ca40, missing rays above 4 MeV, were there in B-VI.8 !!

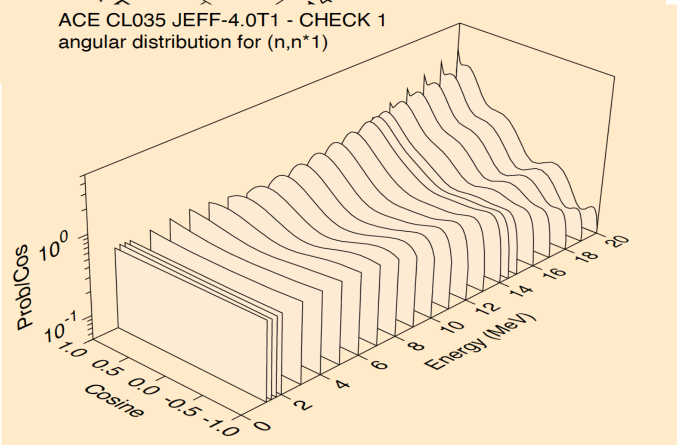


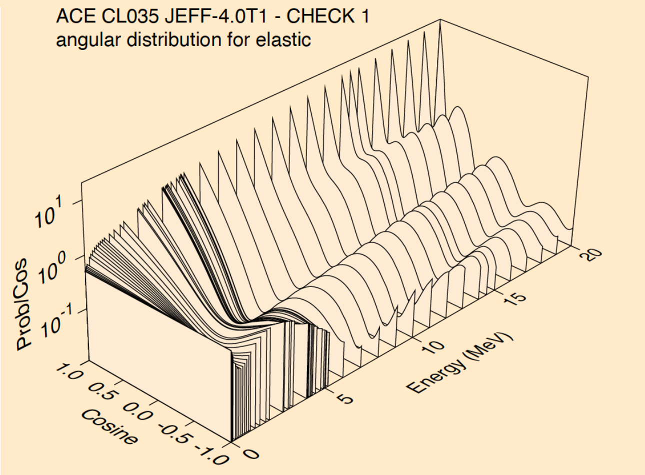
Challenges

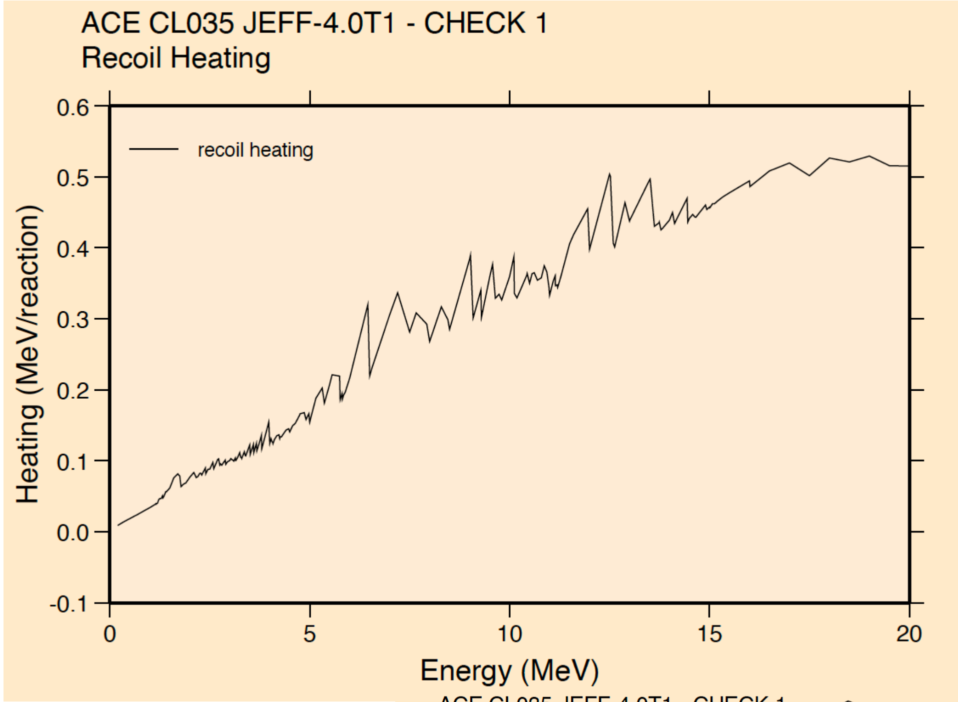
- Issues with ENDF-6 implicit s0 evaluation, explicit/ implicit format transition energy? 30 MeV for TENDL-2021 s30
- GNDS enhancements better satisfy the applications forms landscape
- Processing, what does it means
  - Kalbach-Mann forms direct interpretation in Monte Carlo code
  - PDF, CDF direct interpretation in Monte Carlo code
  - Missing data block for an event, no complete processing possible
  - Multifaceted, mixed forms:
    - widths and averages
    - Legendre and tabulated
    - lines plus continuum
    - etc..
- Are GNDS containers equivalent to hybrid ?

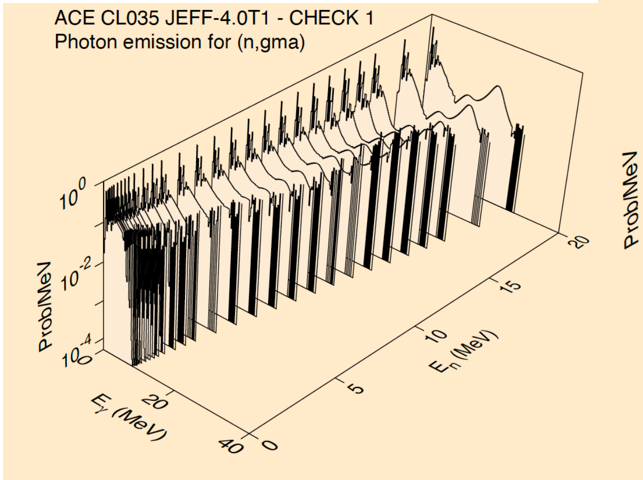
Application forms – beyond cross-sections

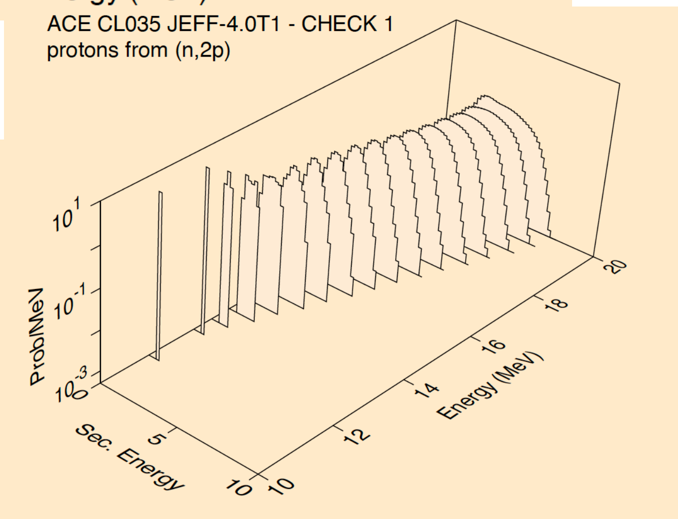




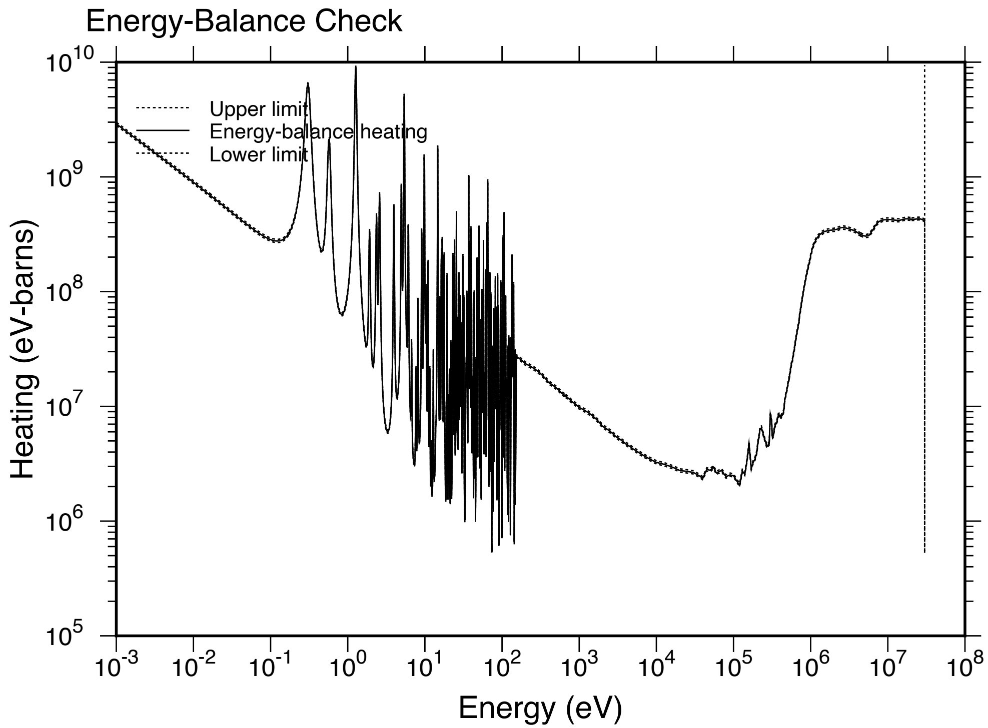


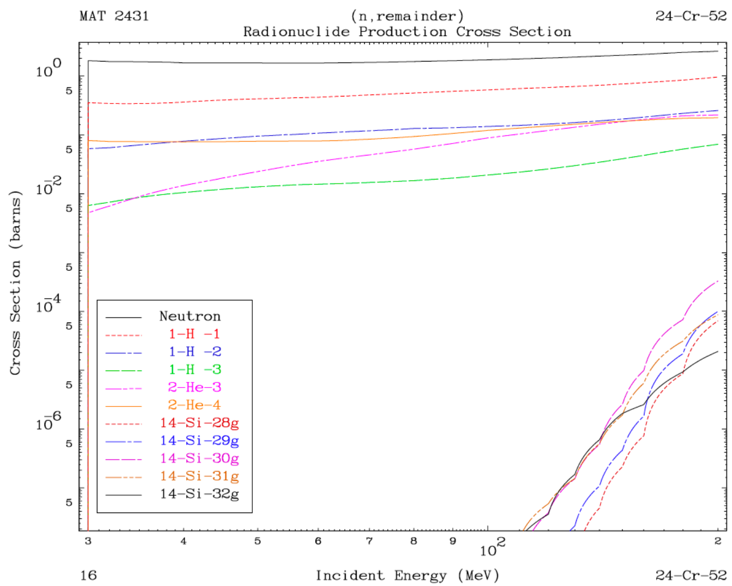


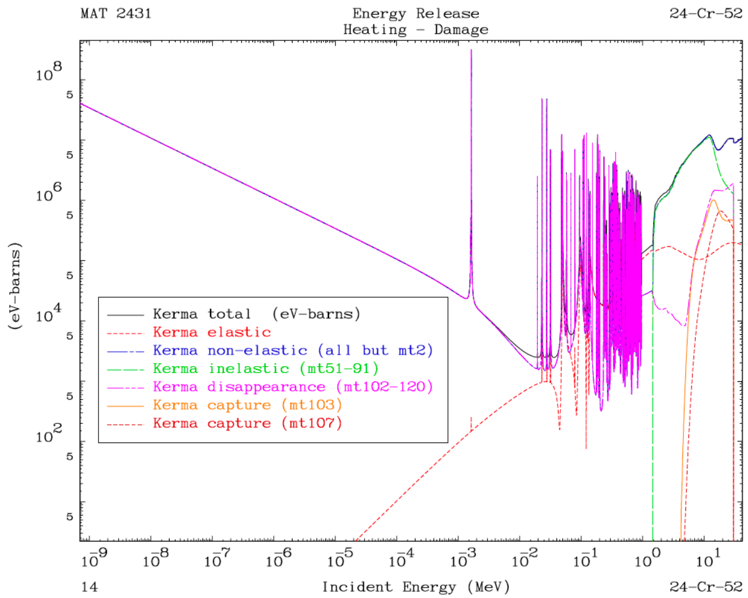


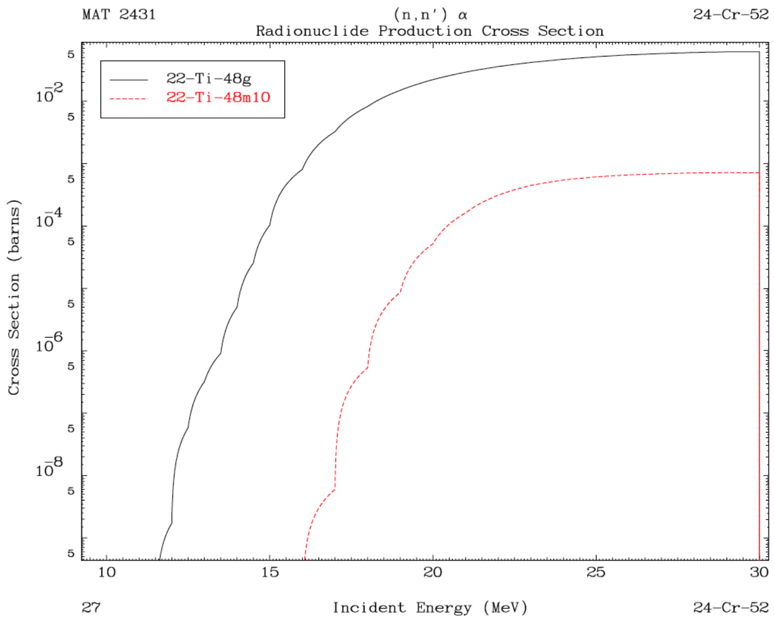


Application forms – beyond cross-sections









Lexical semantics

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

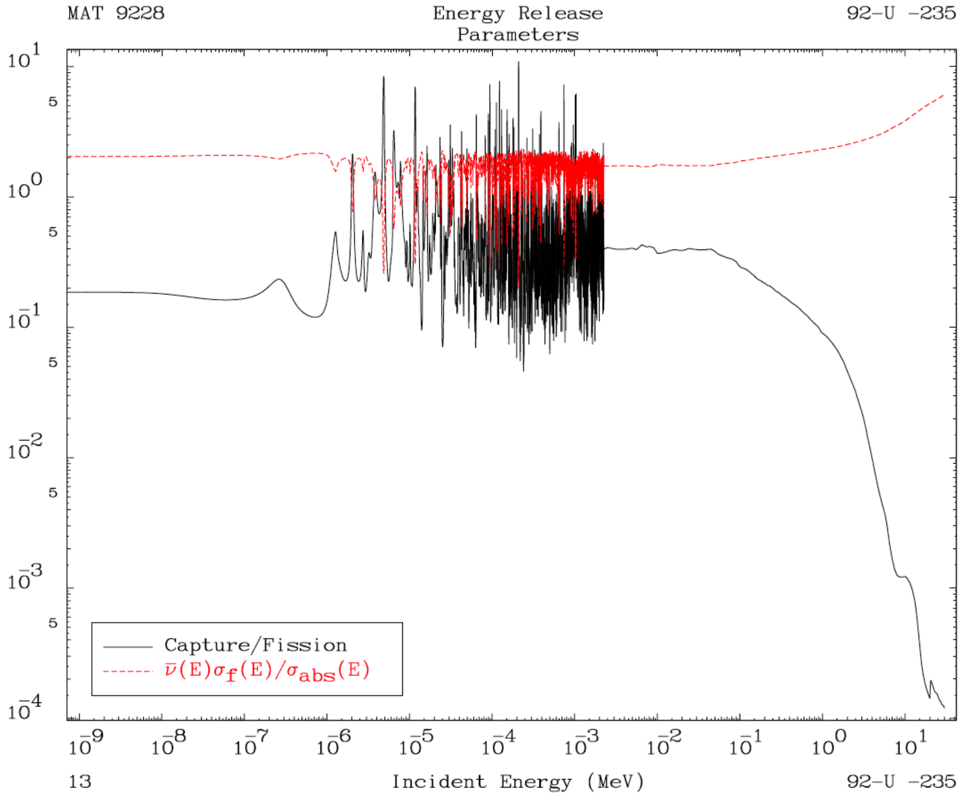
} Structure Format

- Hybrid File >> from PREPRO + NJOY + CALENDF +..
  - derived mt's (gaz, kerma, dpa,…)
  - different data sum rules
  - different applications driven data forms (PKAs, PTs,…)
  - Linearised all the ways

- It is important to differentiate between:

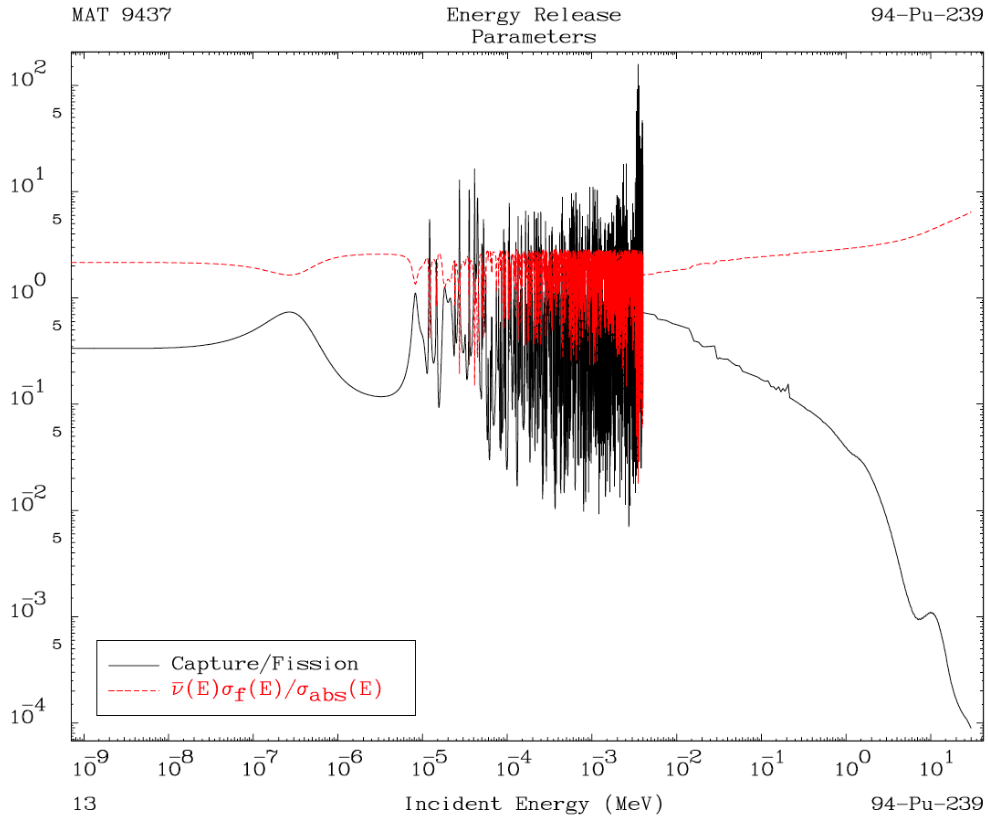
  nuclear data form, format and formalism

Fissile U235 & Pu239 eta and alpha



Simple PREPRO FIXUP run results added to the pendf tape

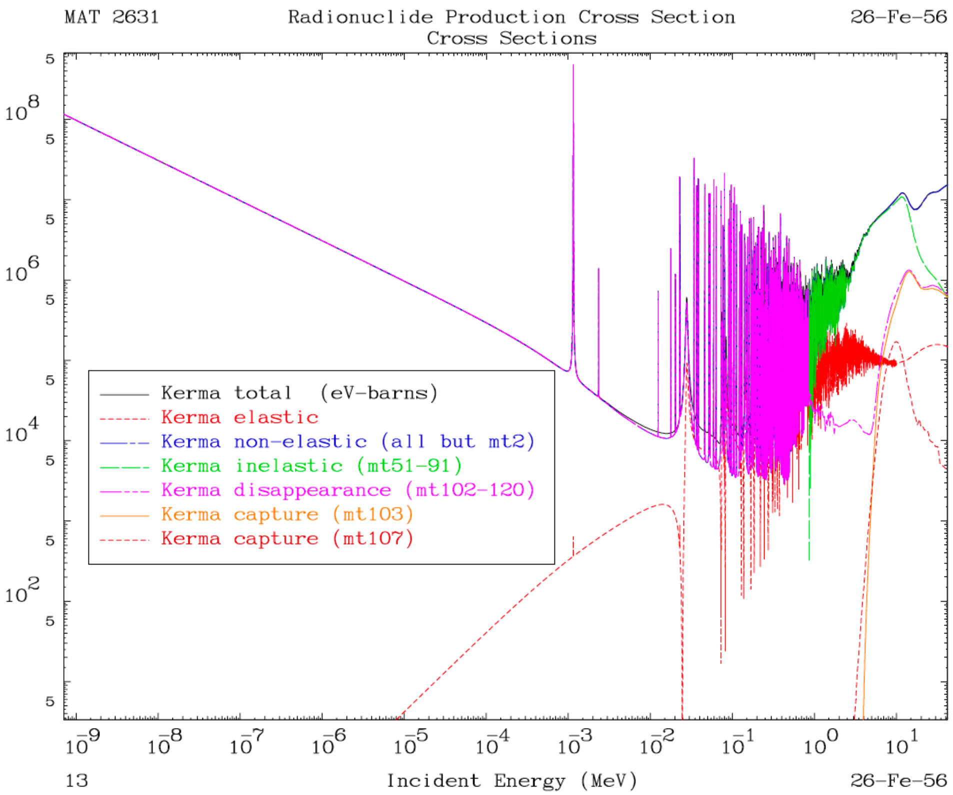
@ Temperature
@ different enrichment

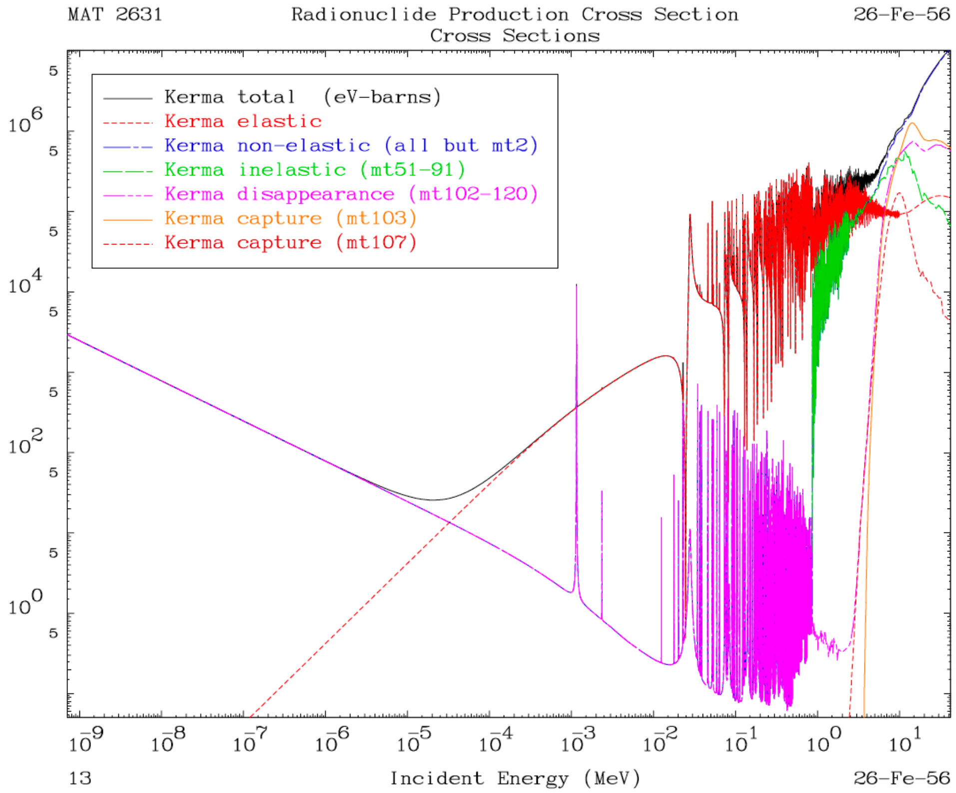


27=(18, 18)+(102,117) **abs.**
333=(452 18) **$\nu.\sigma_f$**
R255=(333/ 27)
R254=(102/ 18) **Capture/fission**

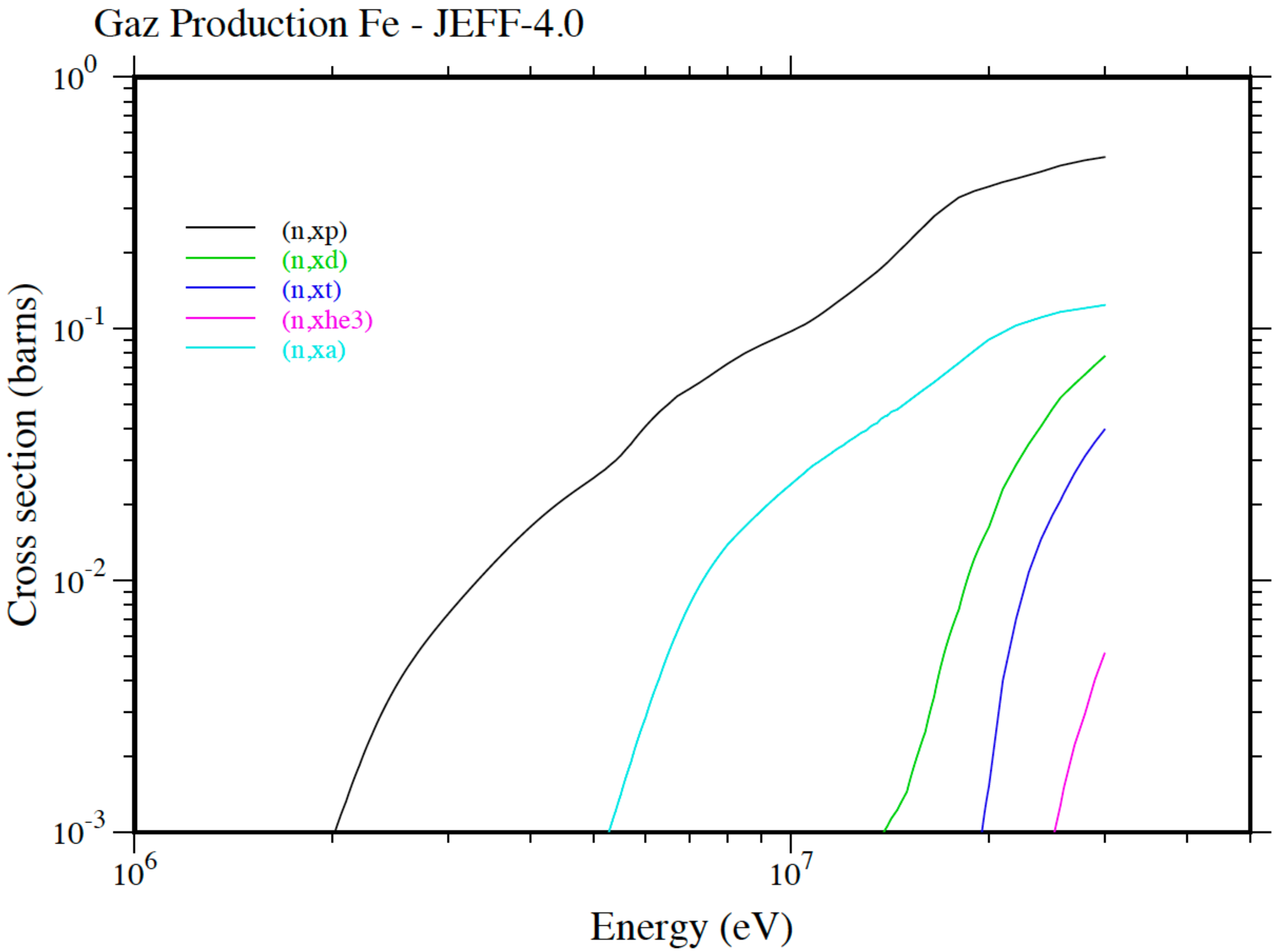
HEATR's KERMA

- Gamma local (FISPACT-II) or transported (MCNP6.3)
- MT's (301 always) 302 303 304 318 401 403 407
- Difference between responses: simulated or build in

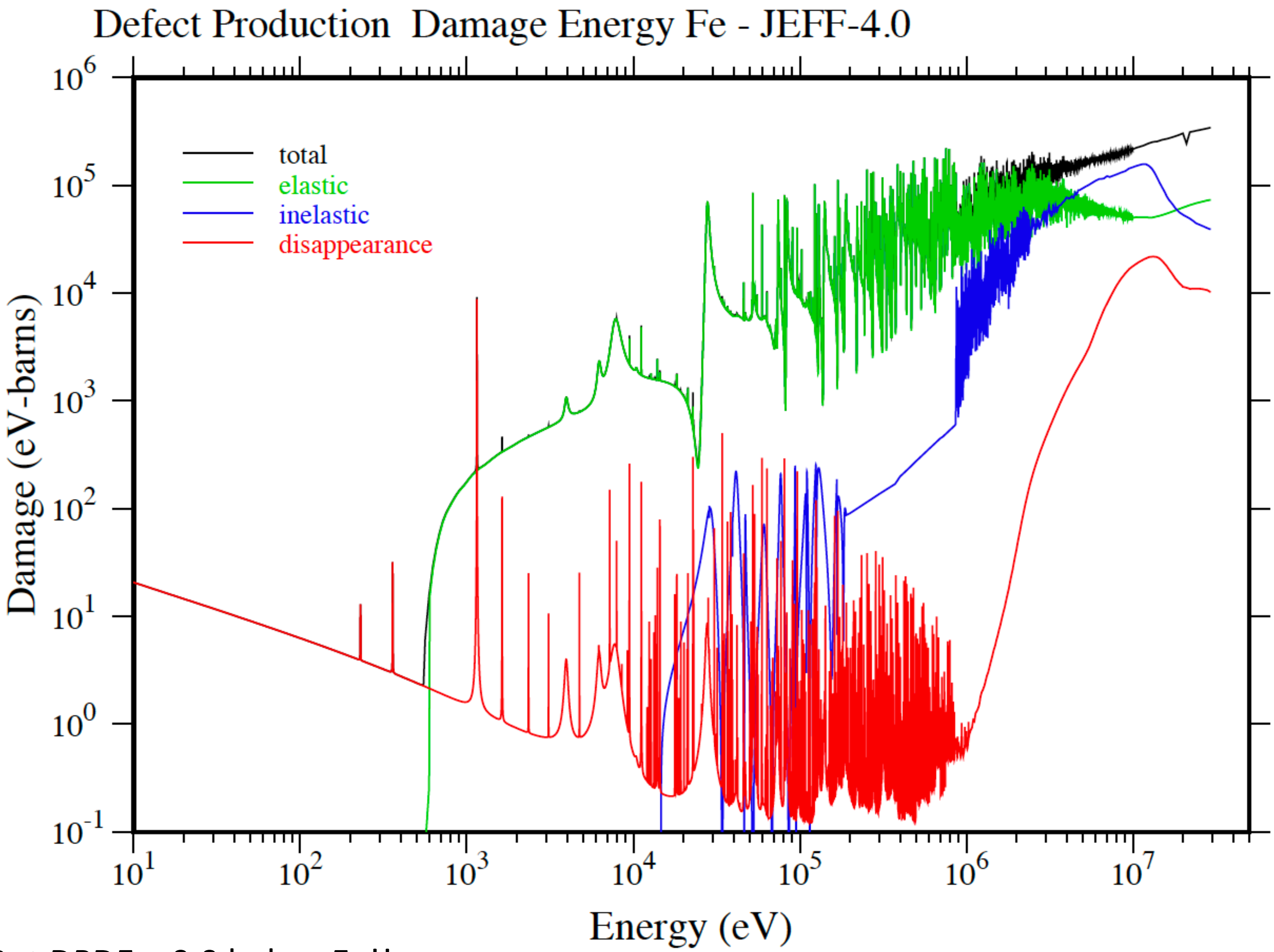




Elemental responses - gaz production

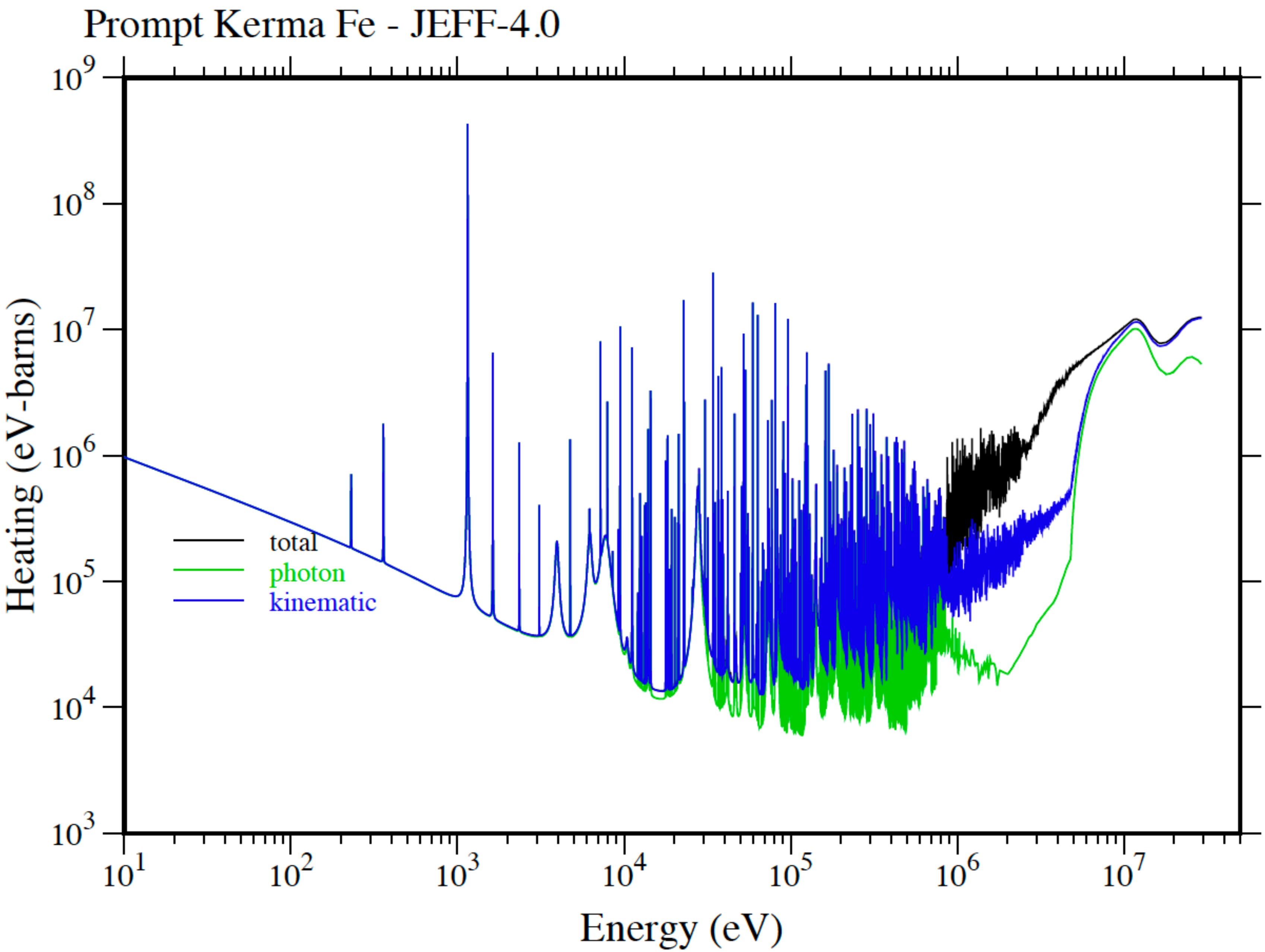


Elemental responses – damage metrics – nothing < E_d



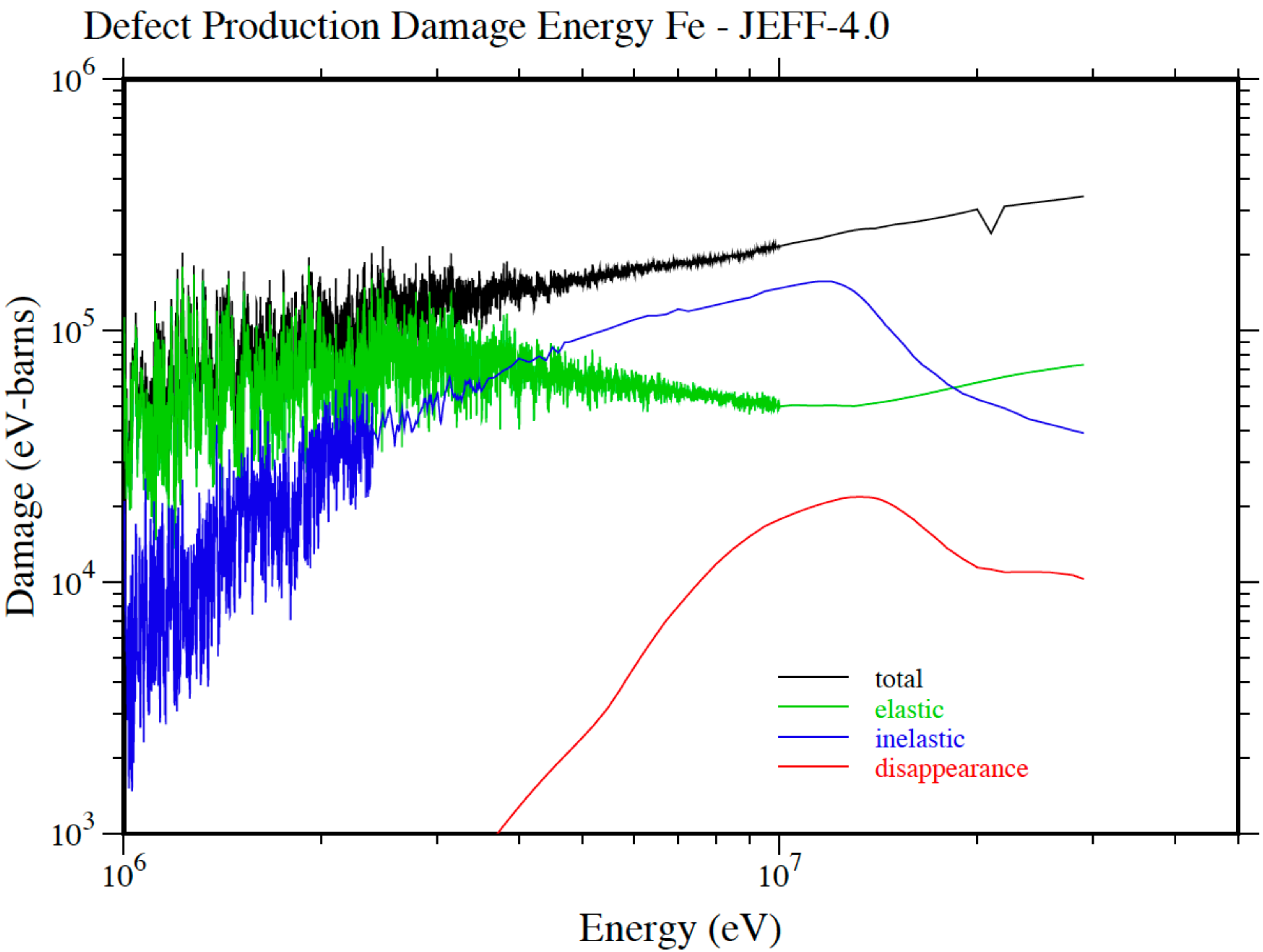
But DPDE = 0.0 below E_d !!

Elemental responses – energy balance/kinematic check



Elemental responses – energy balance/kinematic check

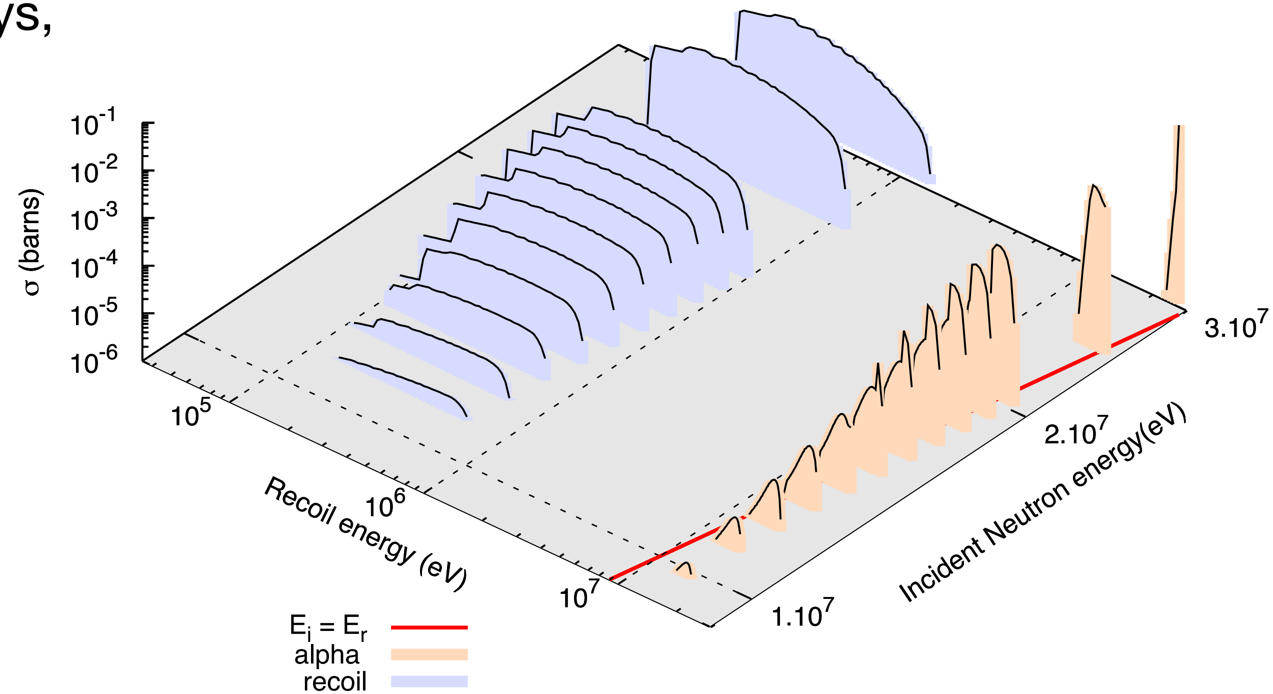
- Zoom in, for fusion technology



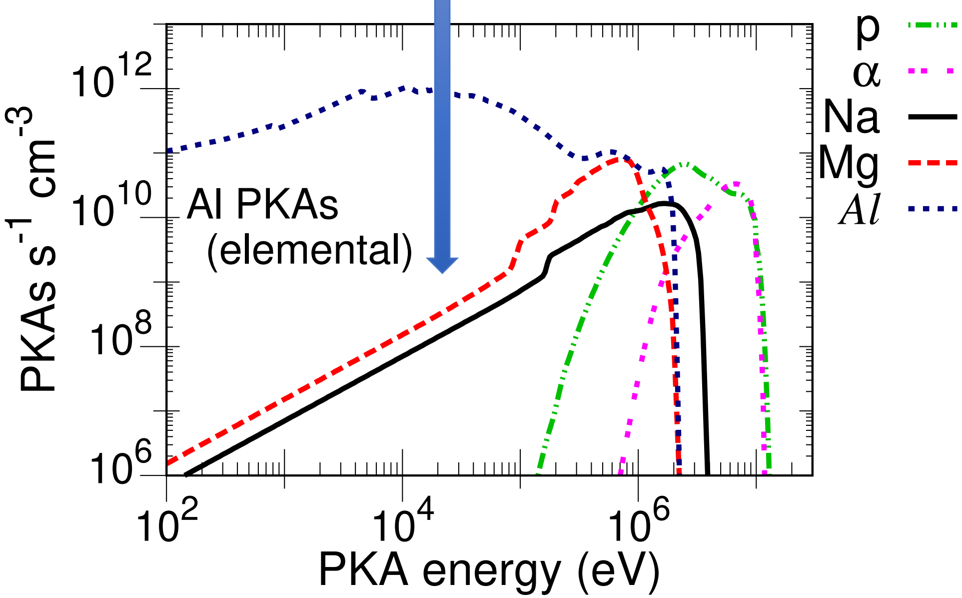
NJOY2016 p, α, residual PKA matrices

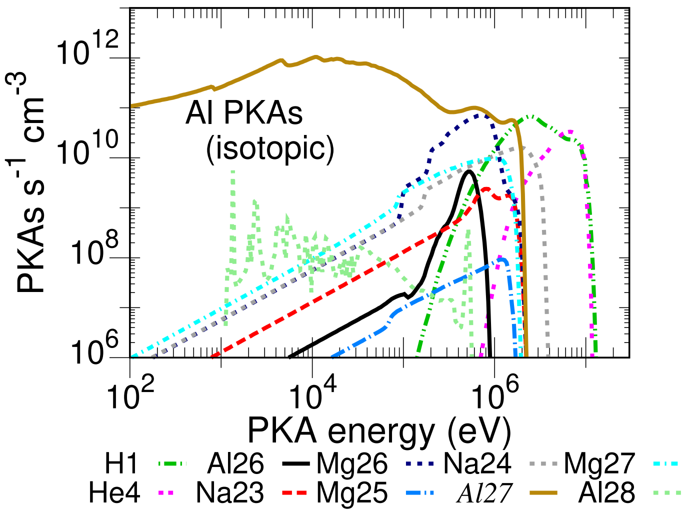
Residual Hf-181 ; $T_{1/2}$=42 days, β- to Ta-181 (stable)

Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the n-incident

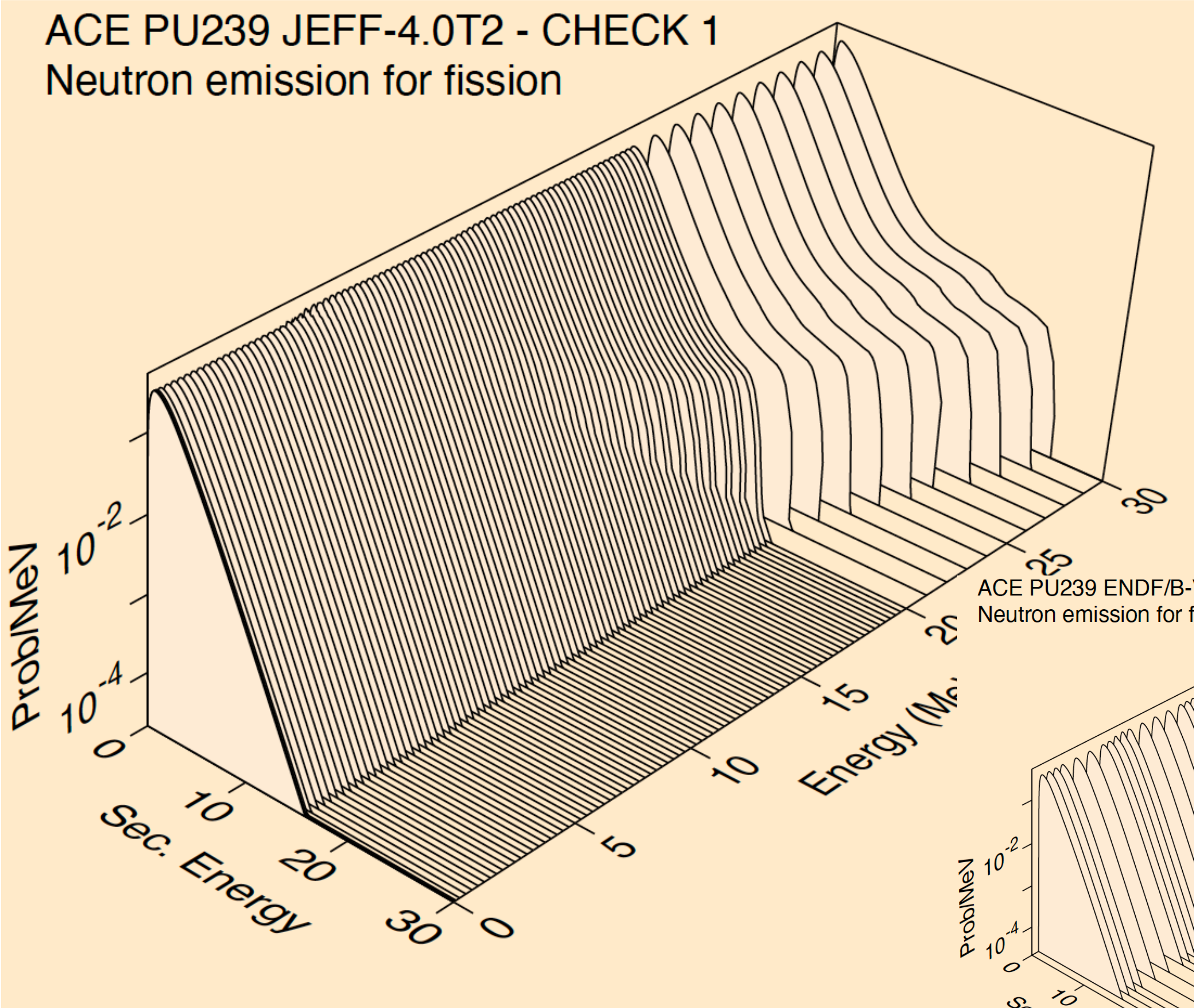


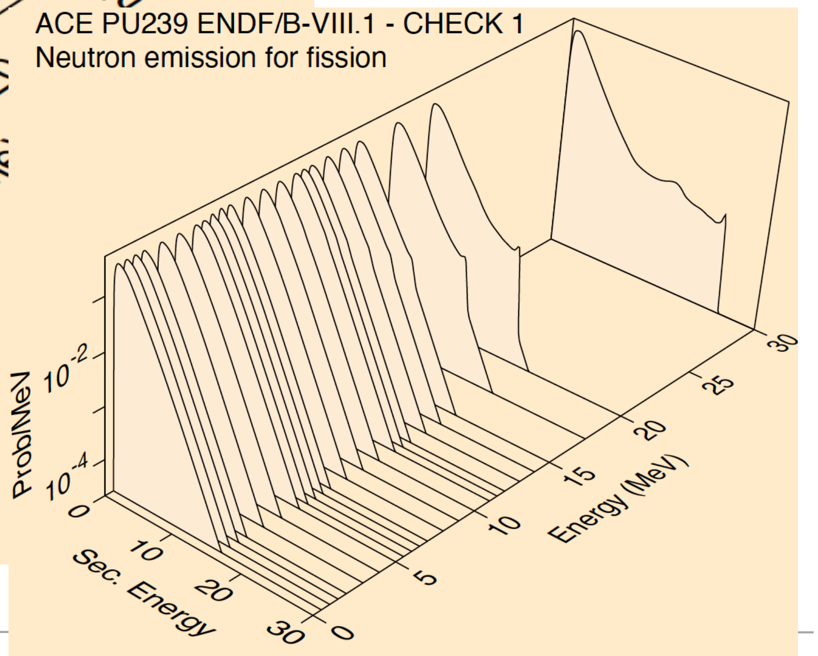
- ismooth





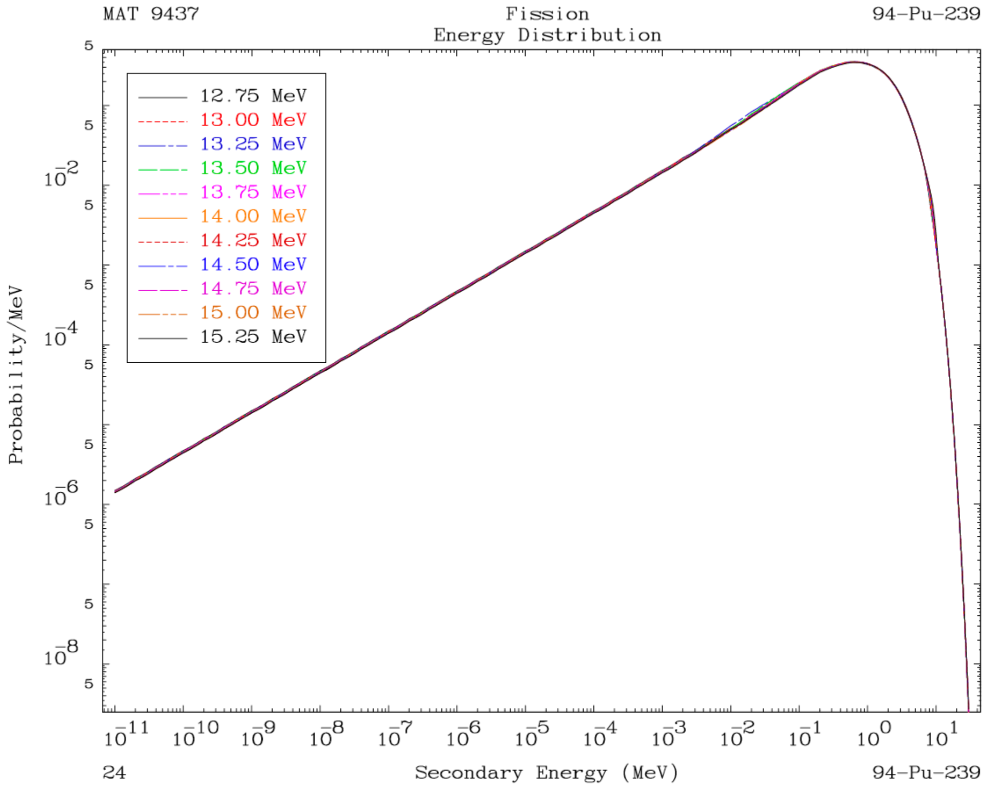
ACE PDF, CDF - neutron emission sec. energy - 3D

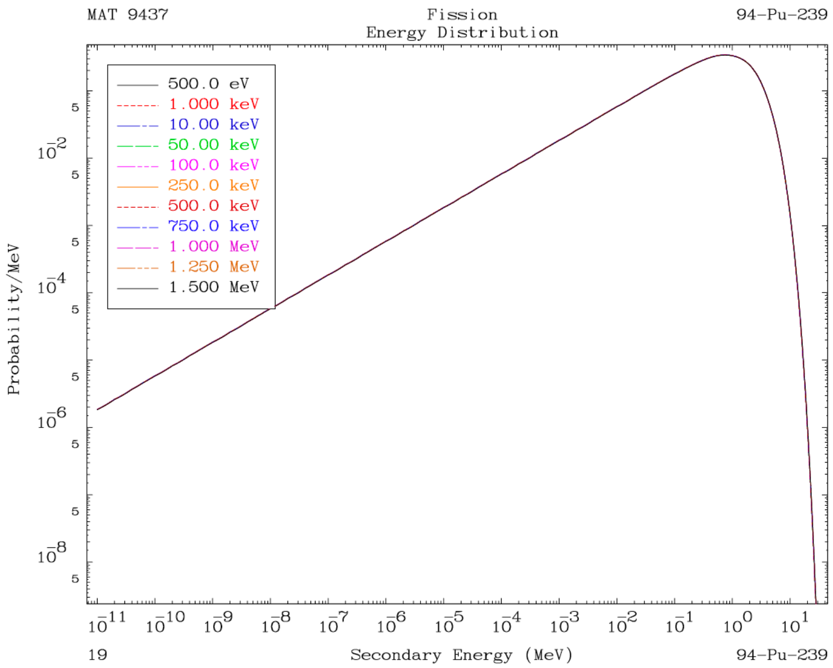


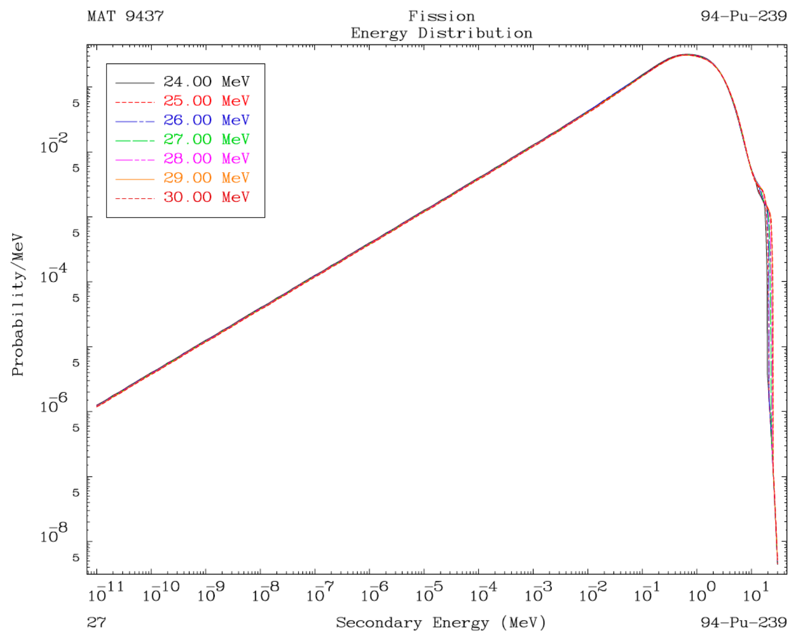


PRE PRO2021- SPECTRA on MF5 - 2D

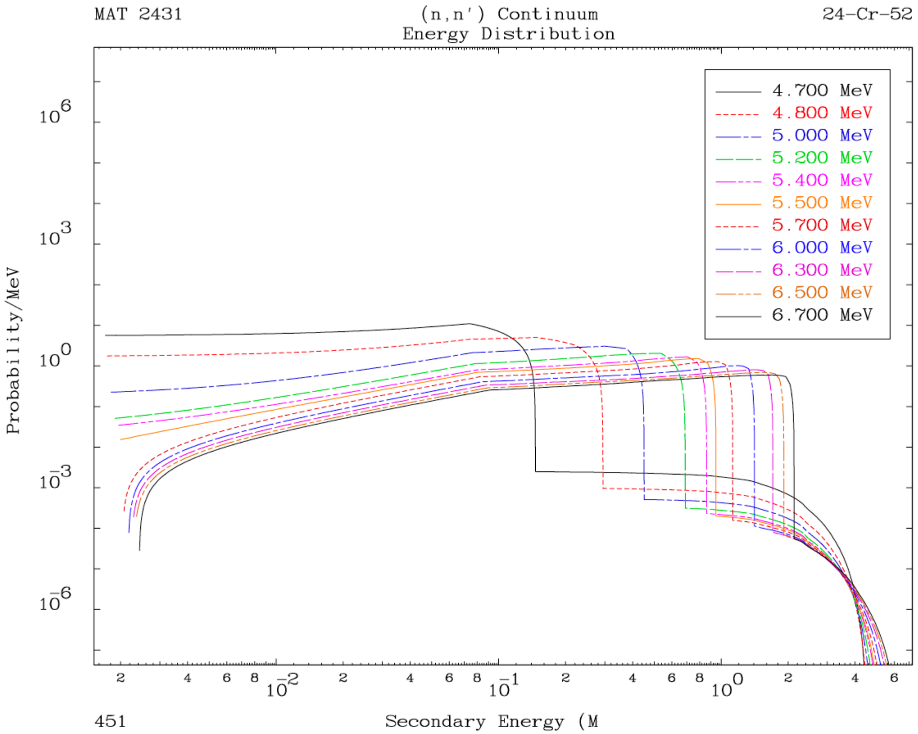
- Tabulates emission spectra

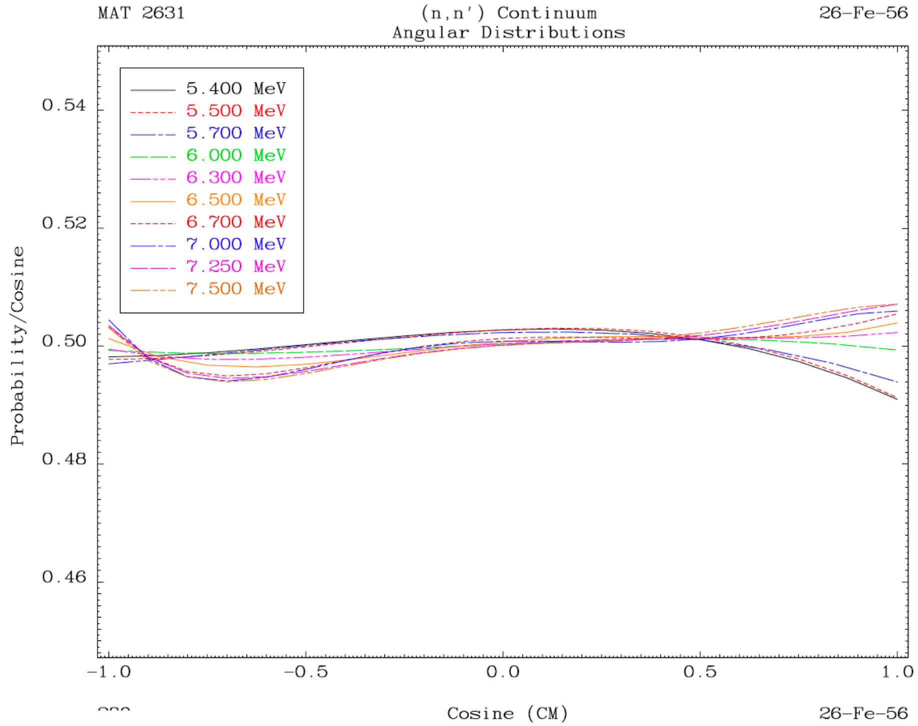


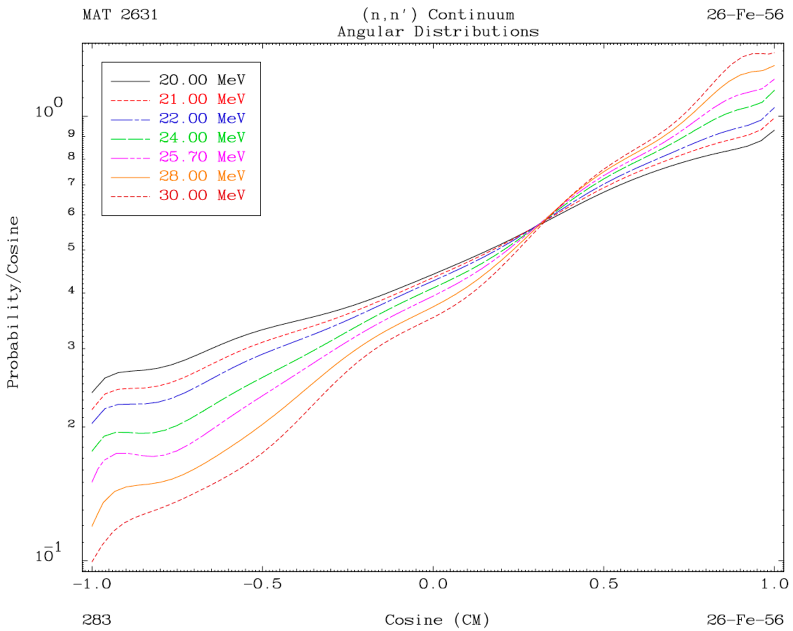




PREPRO2021- SPECTRA on MF5 - 2D

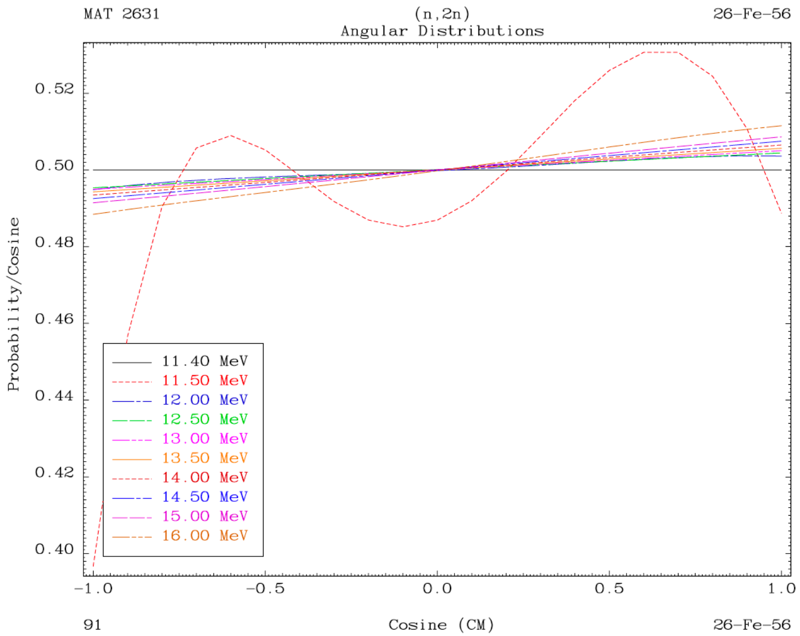


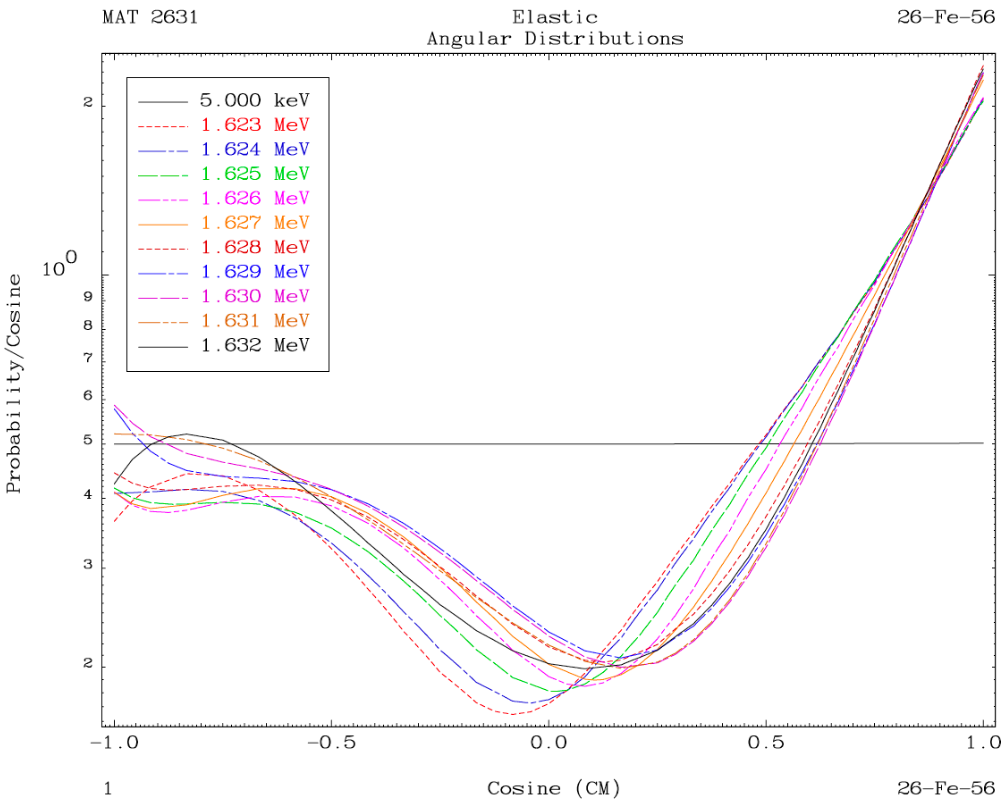


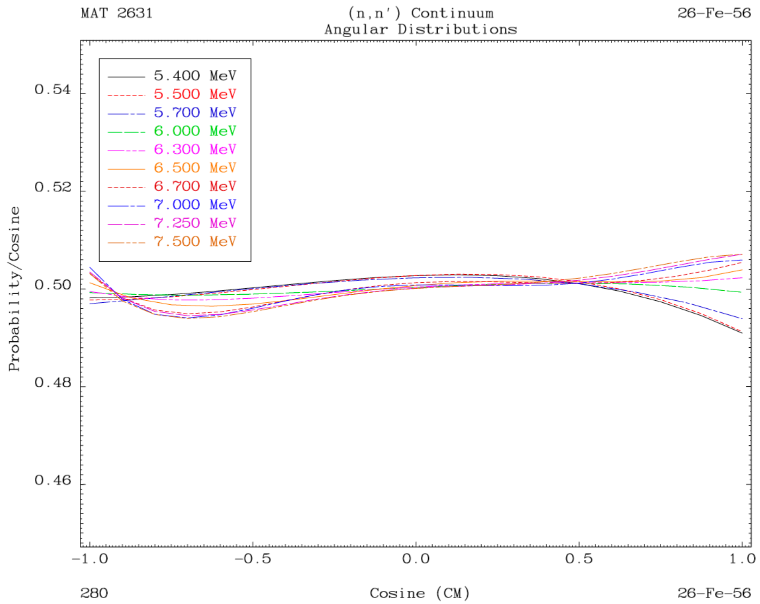


PREPRO2021- LEGEND on MF4 – DD to SD

- convert tabulated angular distributions and Legendre coefficients to lineraly interpolatble tables
- check, clean, curate







Conclusions

- Evaluated forms are just a commencement, although it is seen as an end by an entire community
- The burden of evaluation is the responsibility of the evaluator(s) and/or their institution(s)

- The laws of Physics allow many verification (not validation) processes to take place during processing
- 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 to forms useful for applications and well beyond cross-section or criticality studies only

Thank you for your attention!

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