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NJOY's heatr, gaspr, groupr usage, capability, and limitation

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Lexical semantics

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

} Format

- Hybrid END File >>> from PREPRO 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 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
- ANISO tropy
- A Compact Endf
- Probability Tables
- PDF and CDF
- …

Nuclear data application forms

Formalisms

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

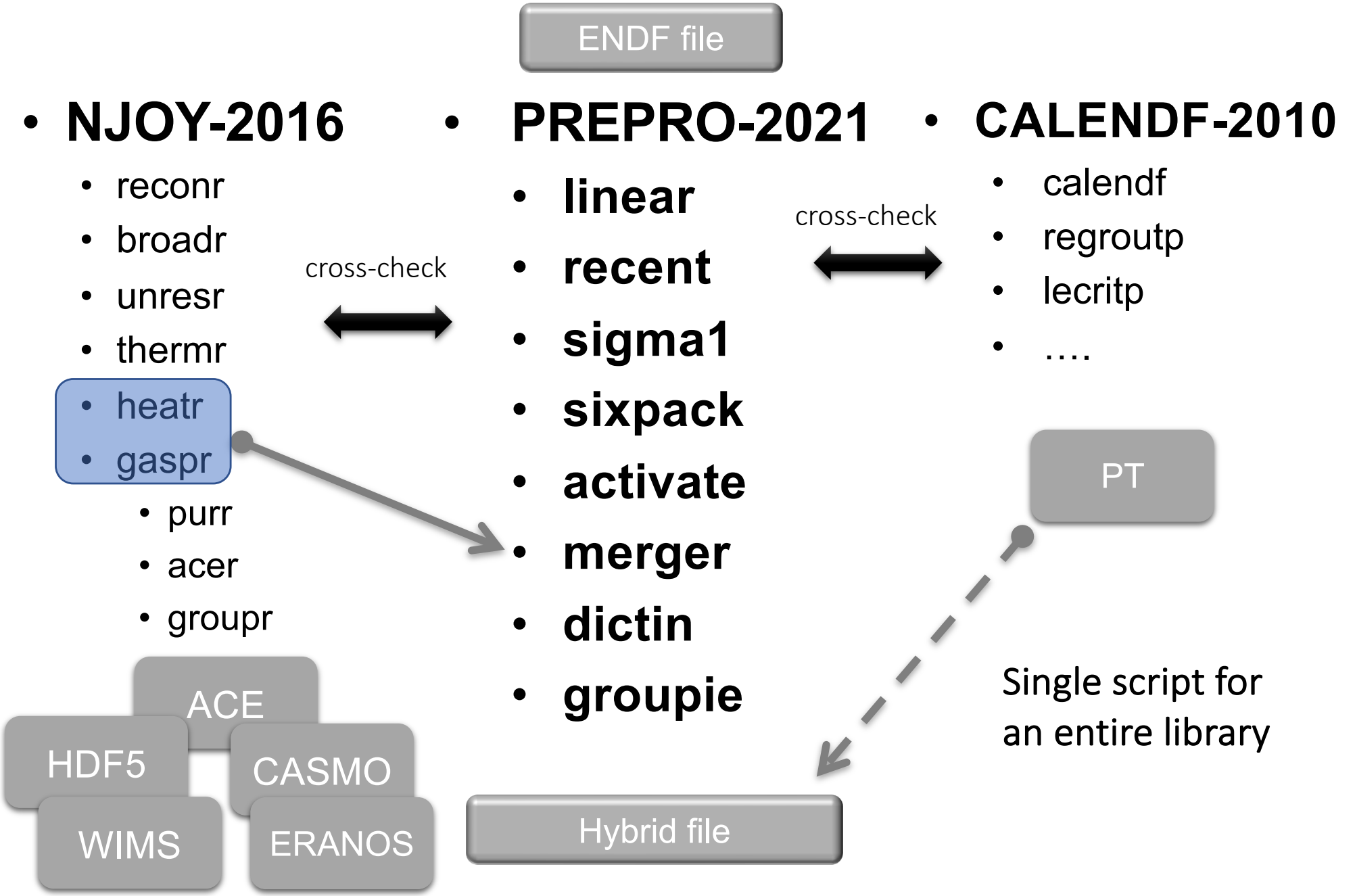
Lexical semantics

- 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, 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

Processing trails: an example with three codes



NJOY2016 HEATR, GASPR, GROUPR

- The NJOY's modules:
  - HEATR for Kerma heating neutron-gamma
  - GASPR for gas production (from explicit ENDF-6 form)
  - GROUPR for matrices (proton, deuteron, triton, He-3, alpha and a>4 residuals)

are unique amongst all other openly available processing codes

- This makes the application forms they compute also unique

NJOY-2016 HEATR & GASPR

- The HEATR modules generates pointwise heat production cross sections and radiation damage energy production for specified reactions and add them to an existing pendf tape
- Heating is often describd by KERMA Kinetic Energy Release in Materials, NJOY computes energy-balance KERMA

```
!     mtk       mt numbers for partial kermas desired
!               total (mt301) will be provided automatically.
!               partial kerma for reaction mt is mt+300
!               and may not be properly defined unless
!               a gamma file for mt is on endf tape.
!               special values allowed—
>                 302   elastic
!                 303   non-elastic (all but mt2)
!                 304   inelastic (mt51 thru 91)
!                 318   fission (mt18 or mt19, 20, 21, 38)
!                 401   disappearance (mt102 thru 120)
!                 442   total photon ev-barns
!                 443   total kinematic kerma (high limit)
```

NJOY-2016 HEATR & GASPR

- The code uses the energy balance method where photon files are available and deposits all photon energy locally when files are not available
- This assures consistency between neutron heating and energy deposition by subsequent photon interactions
- An exception is made for capture where recoil is computed by momentum conservation (mf6 not given for residual)
- Photon files are used to estimate the average photon momentum when available
- A diagnostic message is printed if the momentum calculation leads to a significant error in energy conservation
- Single alpha and proton emission are also partially handled

NJOY-2016 HEATR & GASPR

- maximum 7 responses per HEATR run
  - but then use 2 HEATR runs
- maximum 25 if total kinematic (443 is not asked)
- gamma heat (0 non local, 1 local)
  - 0 for Monte Carlo, that will transport them
  - 1 for applications that do not transport the gamma
- a subsequent HEATR run overwrite the previous one, and this is very convenient when sequential application forms
- the energy-balance kerma factors can be compared with conservative kinematic limits (set iprint=2).
- iprint 1 (max) is full of interesting information, column format

- HEATR, as its developer, is full of subtility

NJOY-2016 HEATR & GASPR

- https://t2.lanl.gov/nis/data/endf/ebalVII.1/summary.html
- Energy-Balance Tests but for ENDF/B-VII.1

Y-89 Good to 12 MeV, fair above.

Y-90 Good.

Y-91 No gammas.

Zr-90 Good below 4.5 Mev, fair above.

Zr-91 Fairly good except only fair from 10 to 15 MeV.

Zr-92 Fair above 3 MeV. Negative kermas.

Zr-93 No gammas.

Zr-94 Fair to poor above 3 MeV. Negative kermas

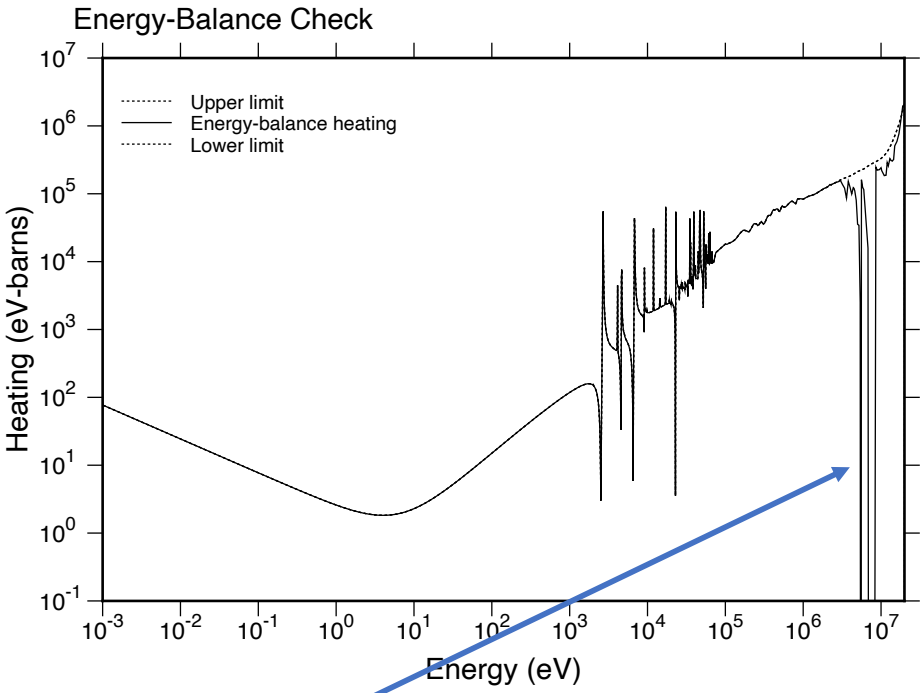
Zr-95 No gammas.

Zr-96 Fair to poor above 3 MeV. Negative kermas.

Nb-93 Nb-93-expanded Good below 800 keV, poor to 20 MeV. Negative kermas.

Nb-94 No gammas.

Nb-95 No gammas.



NJOY-2016 HEATR & GASPR

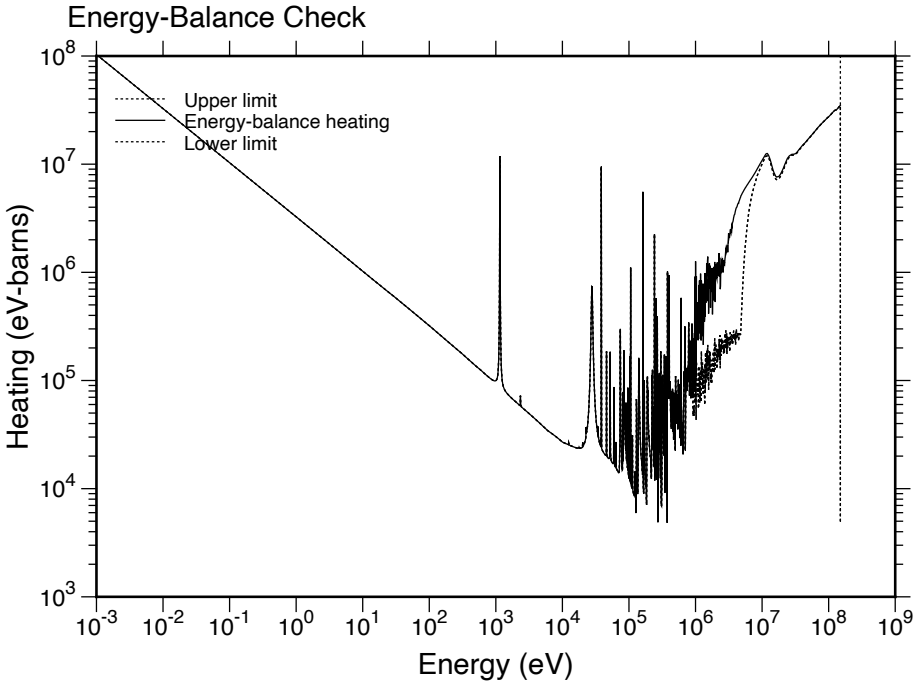
- Computing KERMA by energy balance
  - Not all emitted photon production are given explicitly, summation rules as nonelastic (MT=3) and inelastic (MT=4) is often used
  - MT=18 is the least of our concern for n or γ heating
  - Heating from MF-4, MF-5 and MF-12 (yield data),13 (prod. xs),14 (angle dist), 15 (continuous energy spectra)
  - Heating from MF-6
    - KM need conversion to lab frame
    - Two-body kinematic only !!!
    - Recoil distribution, not always present
    - ..
    - If empty, no heating or damage
  - Extreme care need to be taken for photon and neutron yields and average energies are consistent.

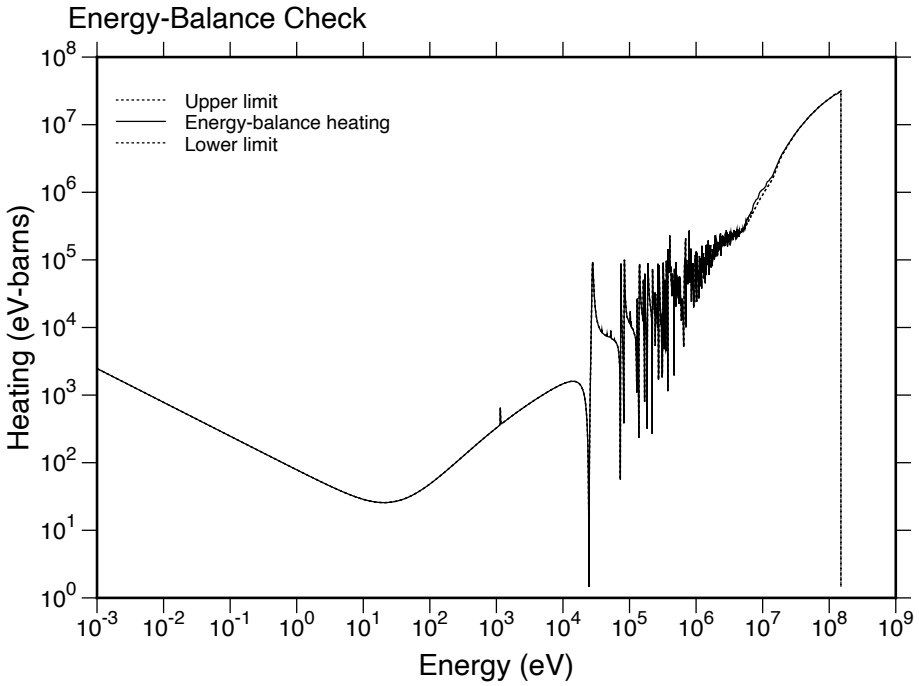
- Computing KERMA from kinematic would requires multi body kinematics and all bodies :entrance, emitted, residual data forms

NJOY-2016 HEATR & GASPR

- Fe056
- 0 non local or 1 local

- Given as an help to evaluator
- Obvioulsy not looked

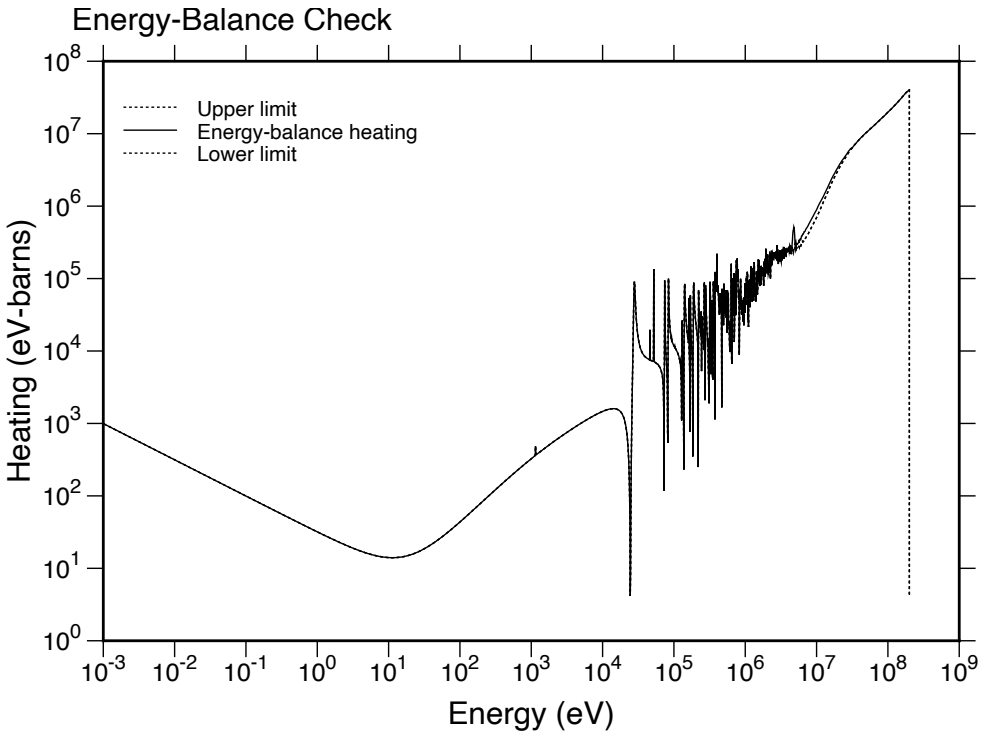


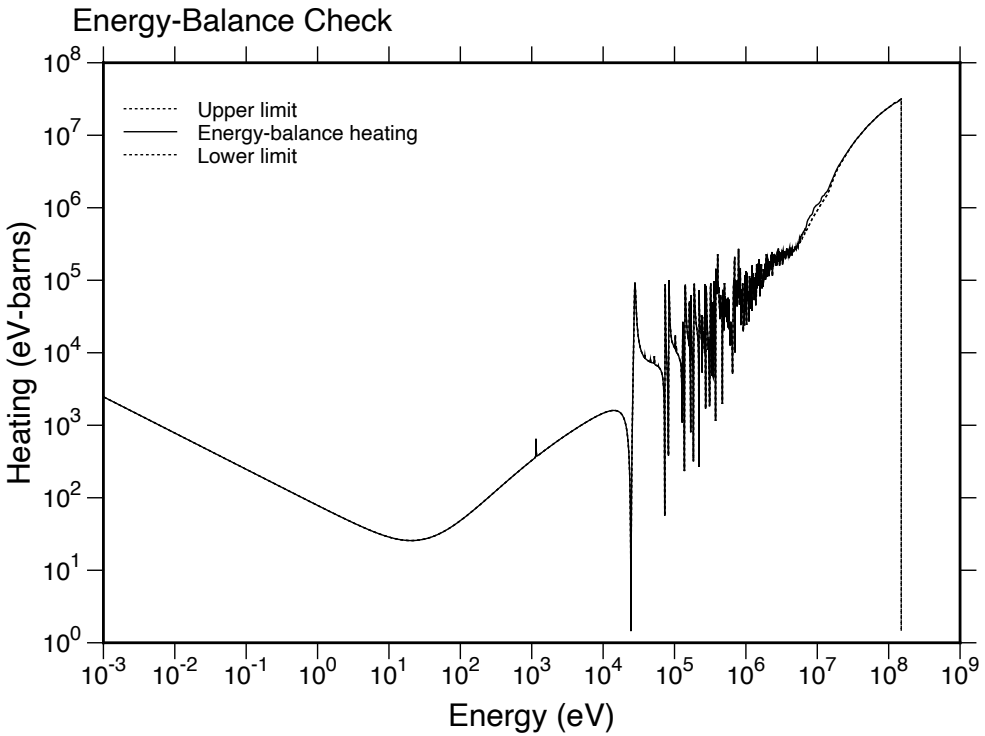


- Obviously the local has some (numeric) issues in the low energy range
- Meaning below say 10 eV ??
- It also show some inconsistancies in the fast > MeV range

NJOY-2016 HEATR & GASPR

- Fe056 TENDL-2021 versuss ENDF/B-VIII.0
- similar shape but rather difference in values

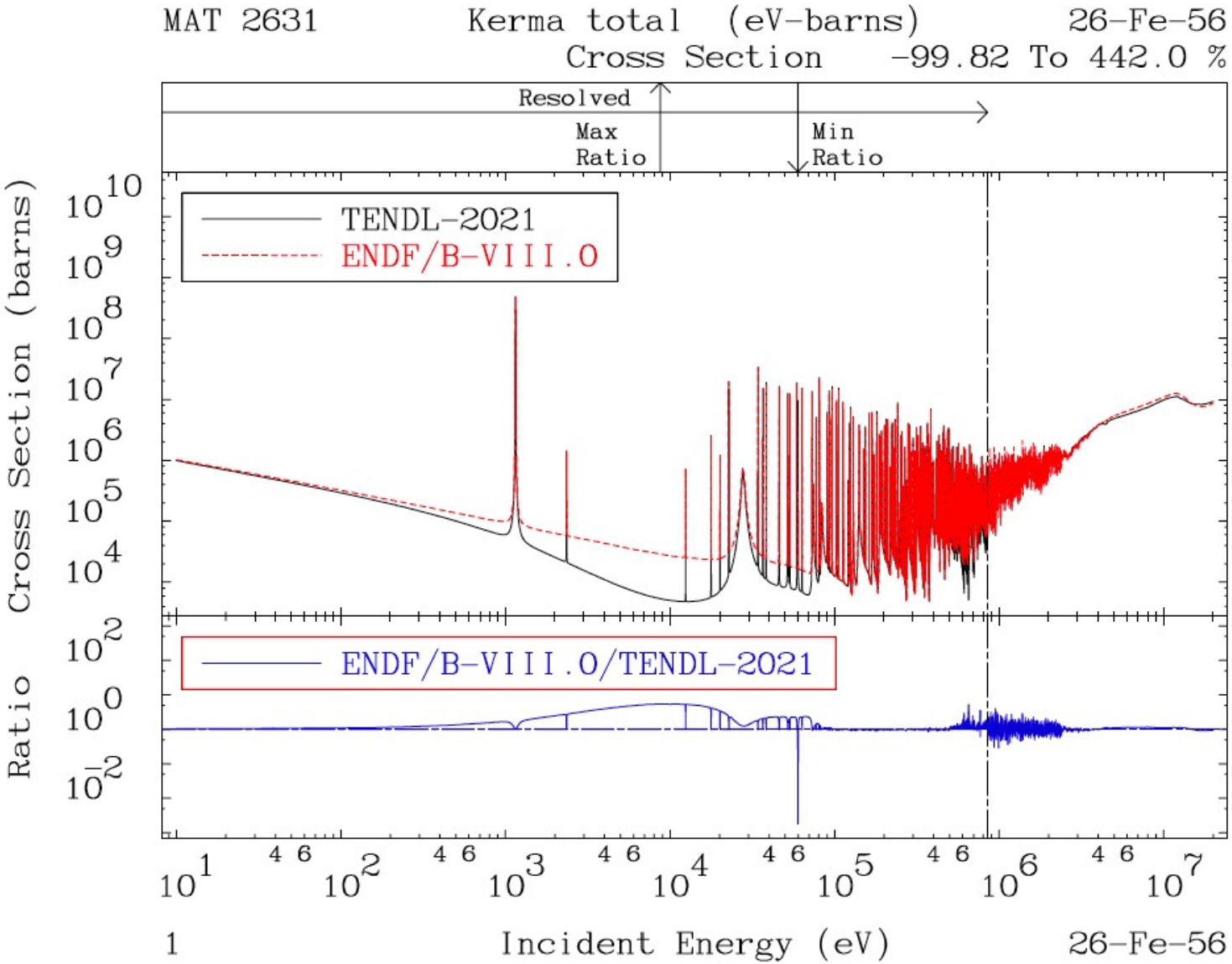




- Are such differences of importance ?
- Are low energy KERMA significant ?

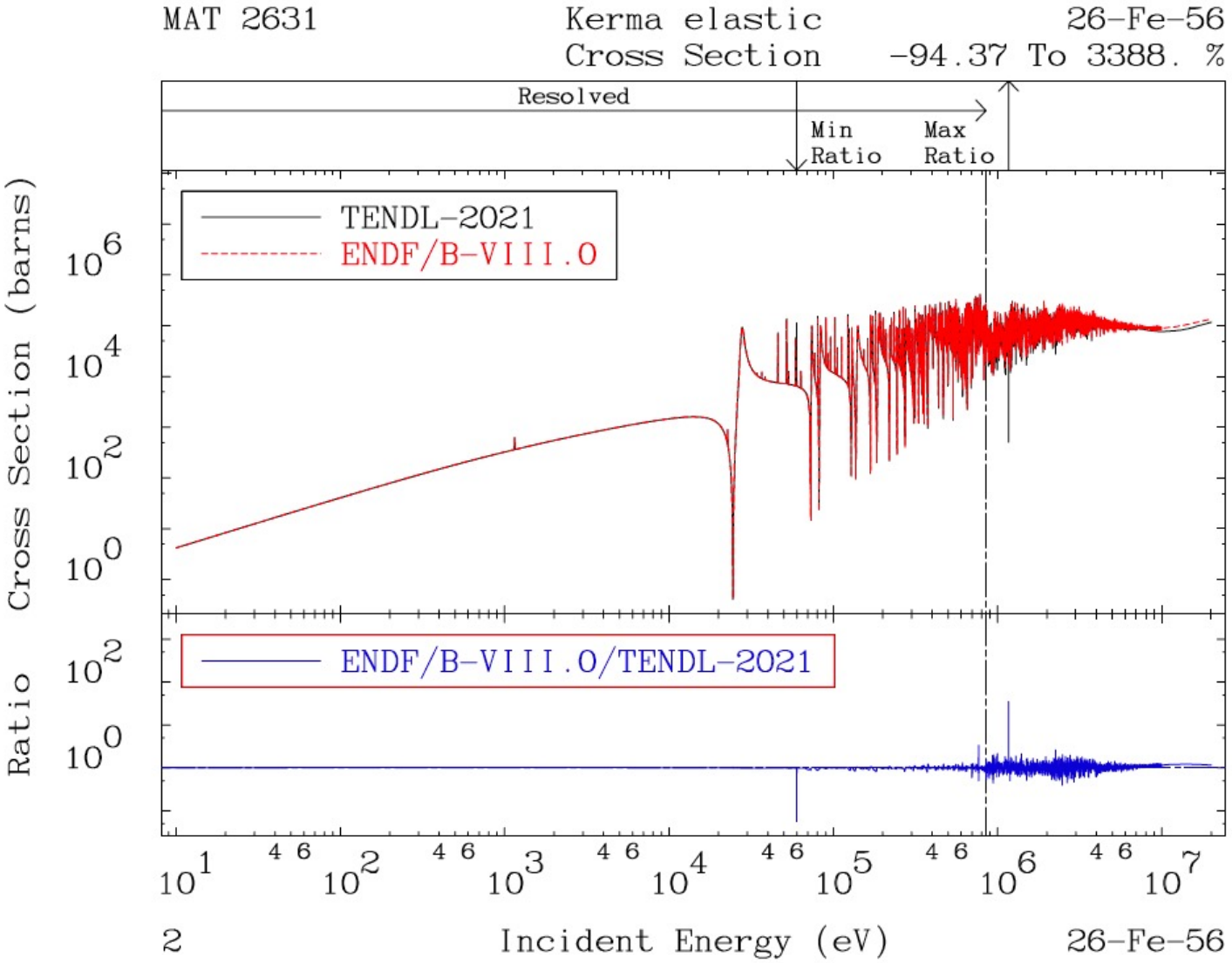
NJOY-2016 HEATR & GASPR

- Difference in the total



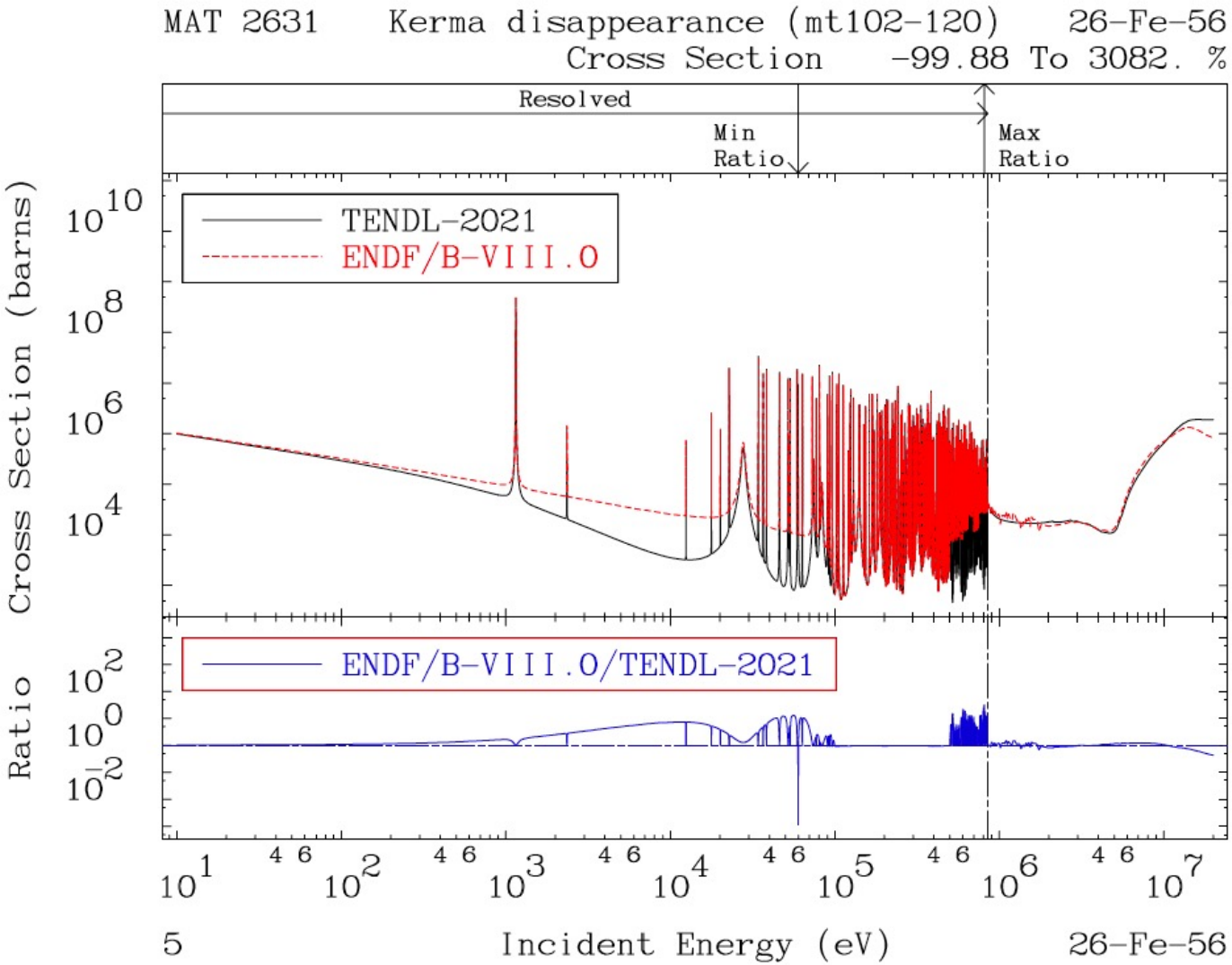
NJOY-2016 HEATR & GASPR

- Not due to the elastic



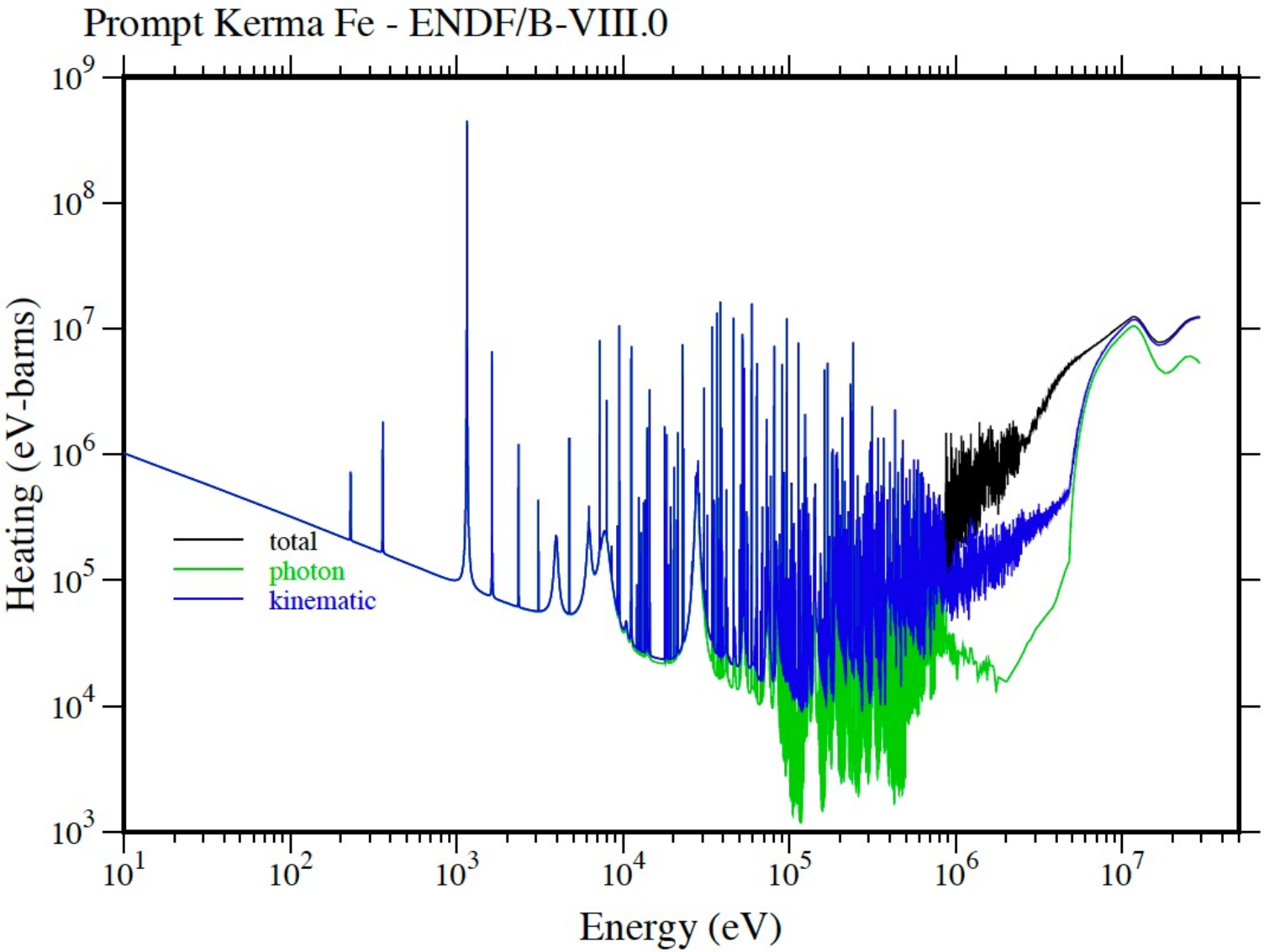
NJOY-2016 HEATR & GASPR

- But the capture, most certainly induced by where the gamma are stored and how they are interpreted

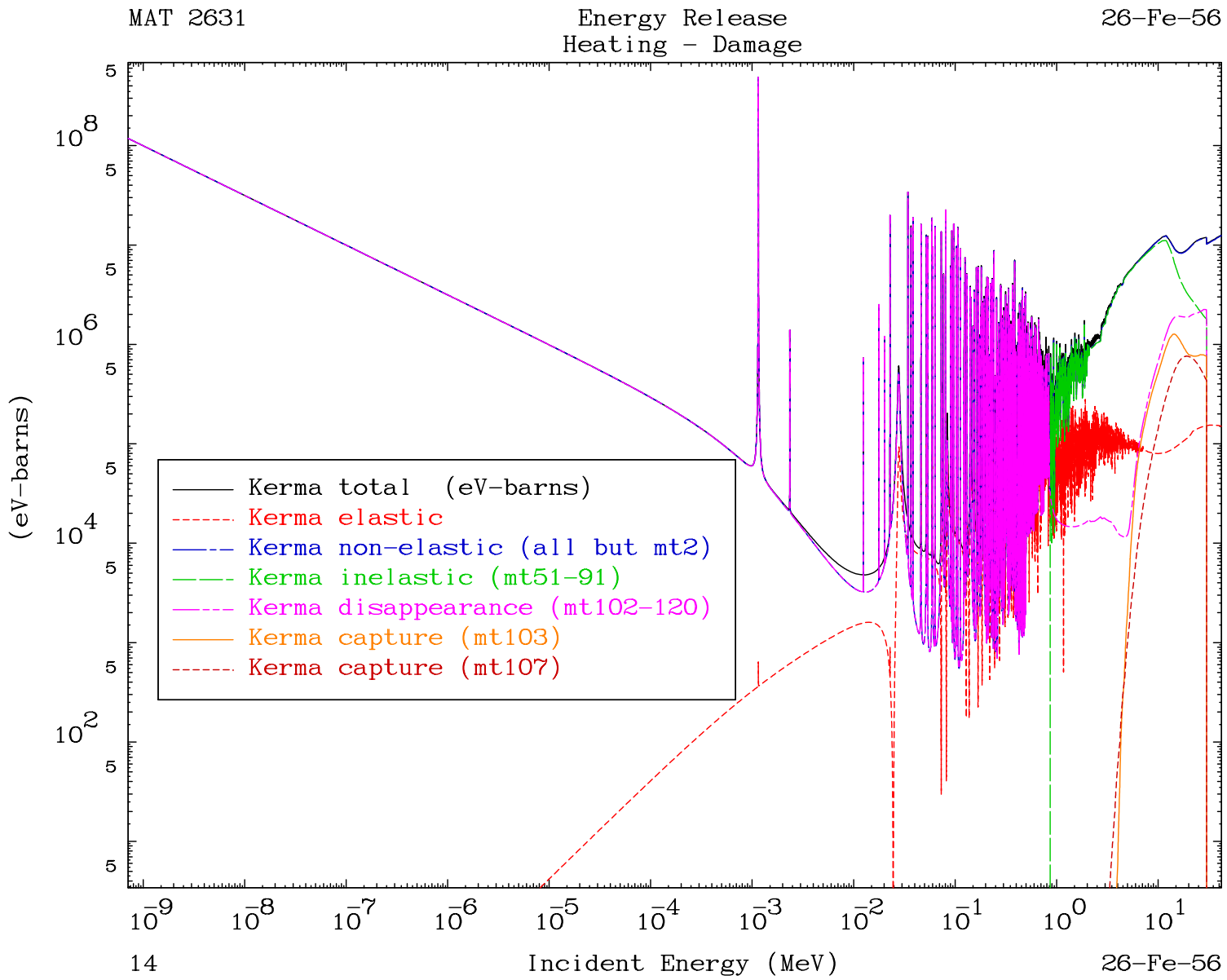


NJOY-2016 HEATR & GASPR

- photon and kinematic KERMA on the element

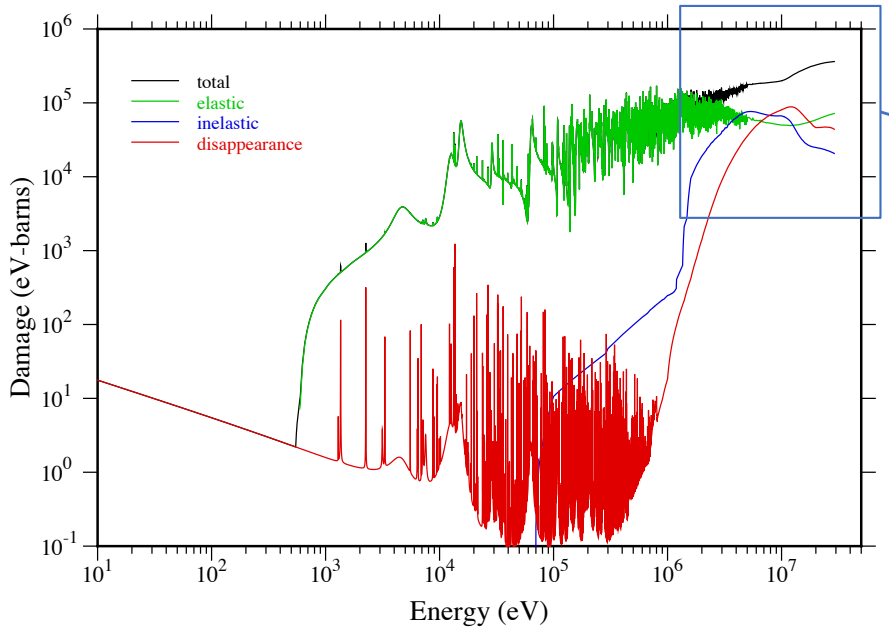


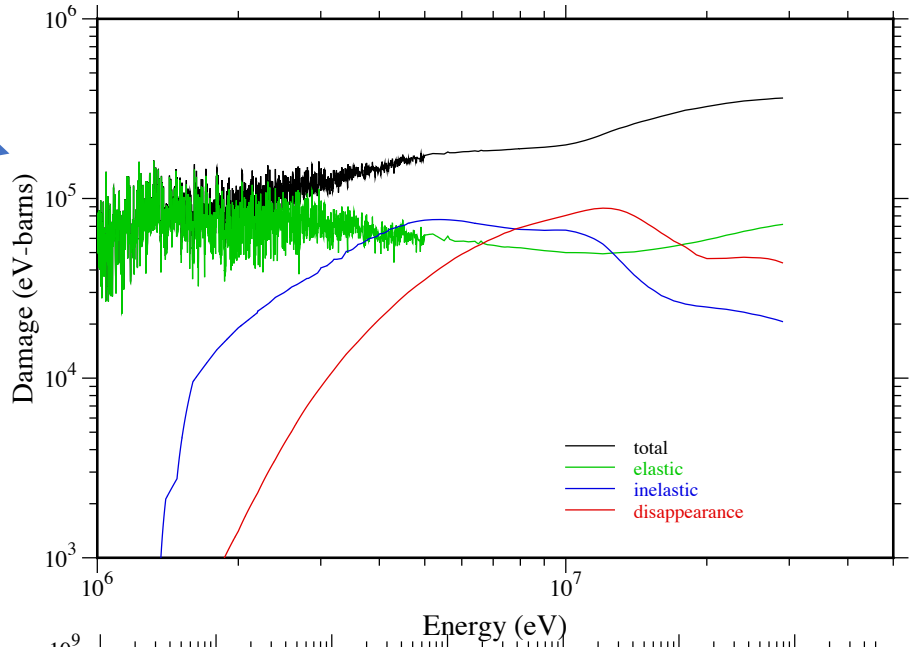
Major, charged particles, heating Kerma, DPA

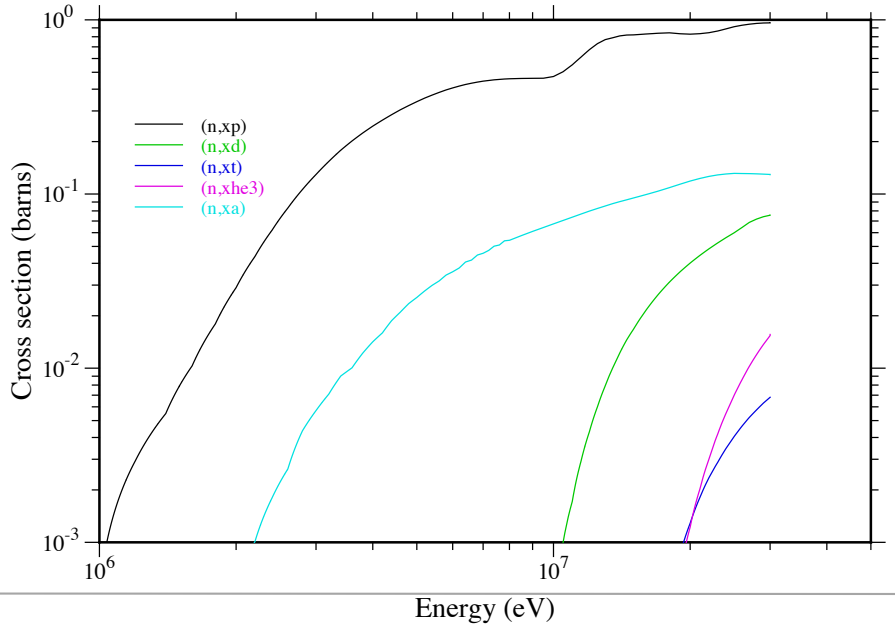


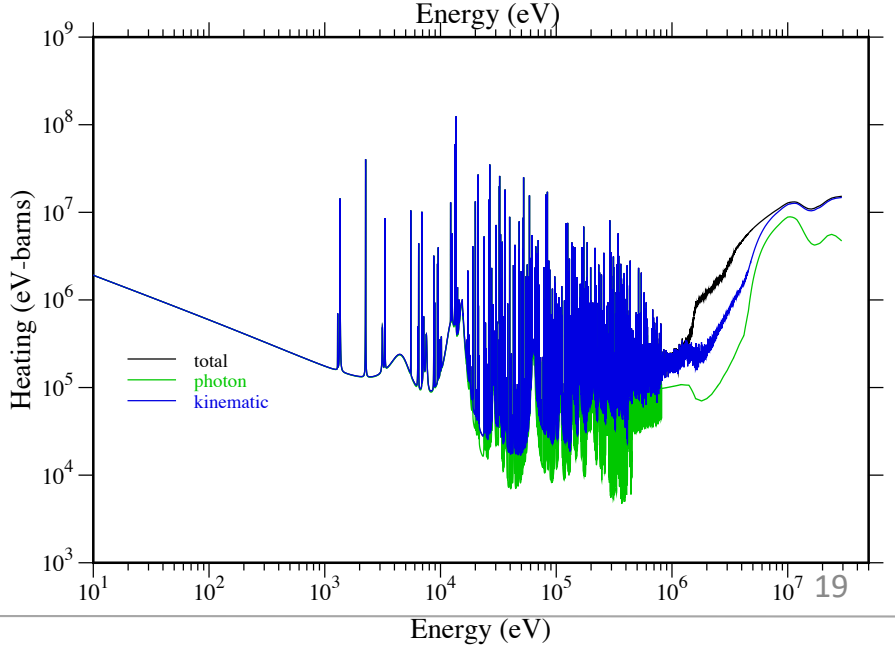
Derived nuclear data forms

- Kerma, Damage Energy, Gas Production (Ni) Elemental



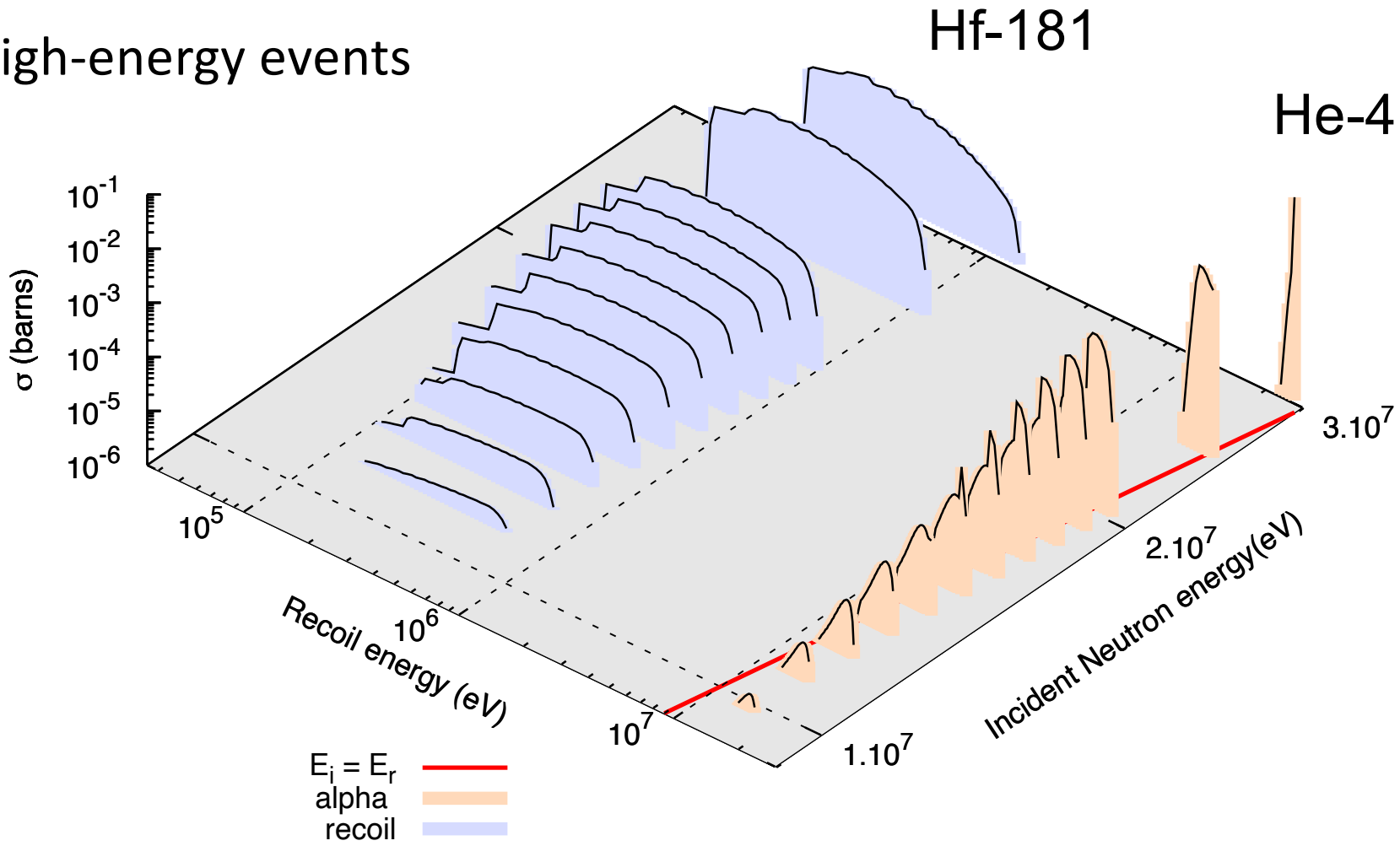






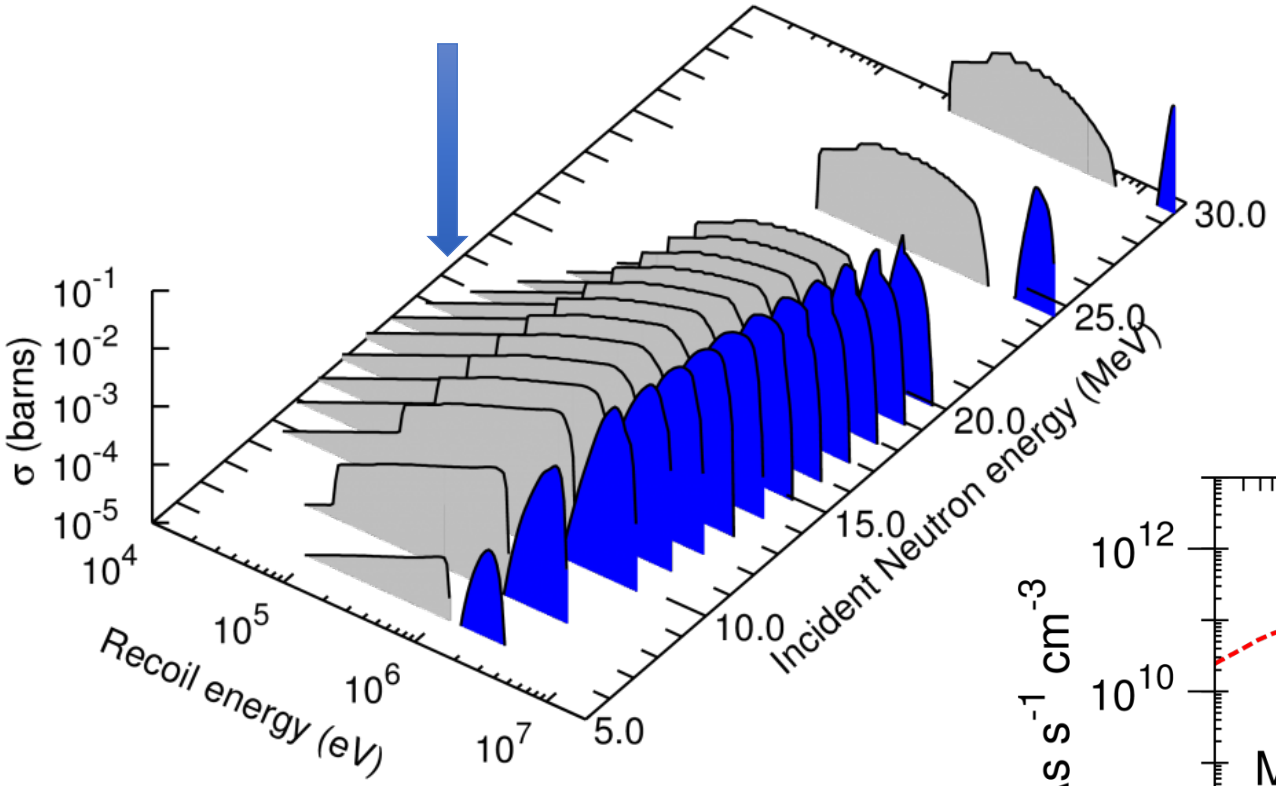
Residual and charged particles matrix

$^{184}W + n$: residual ^{181}Hf - $T_{1/2}$= 42 days, β- to ^{181}Ta (stable)



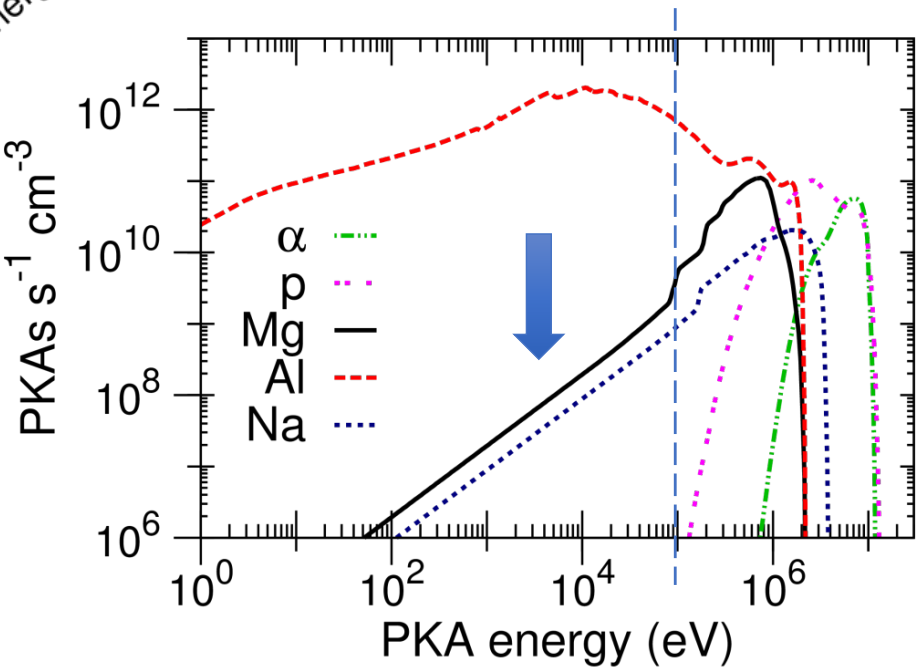
Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the n-incident !!! At 22.7 MeV and above the secondary energy grid is truncated !!!

Matrix NJOY processing ismooth = 1



Tails are important

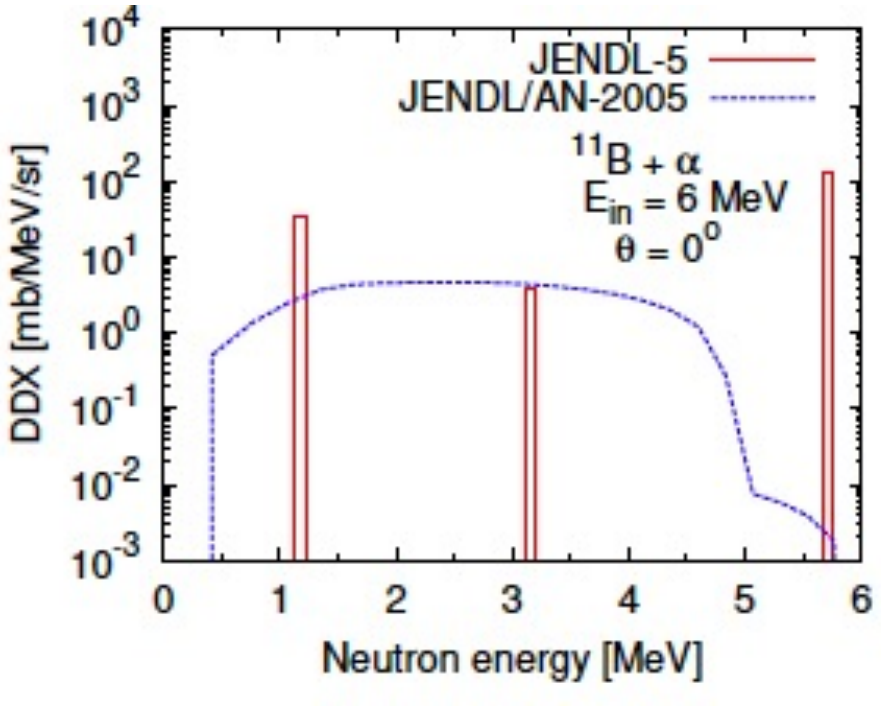
Transmuted residuals also: Mg, Na <u>not Al</u>



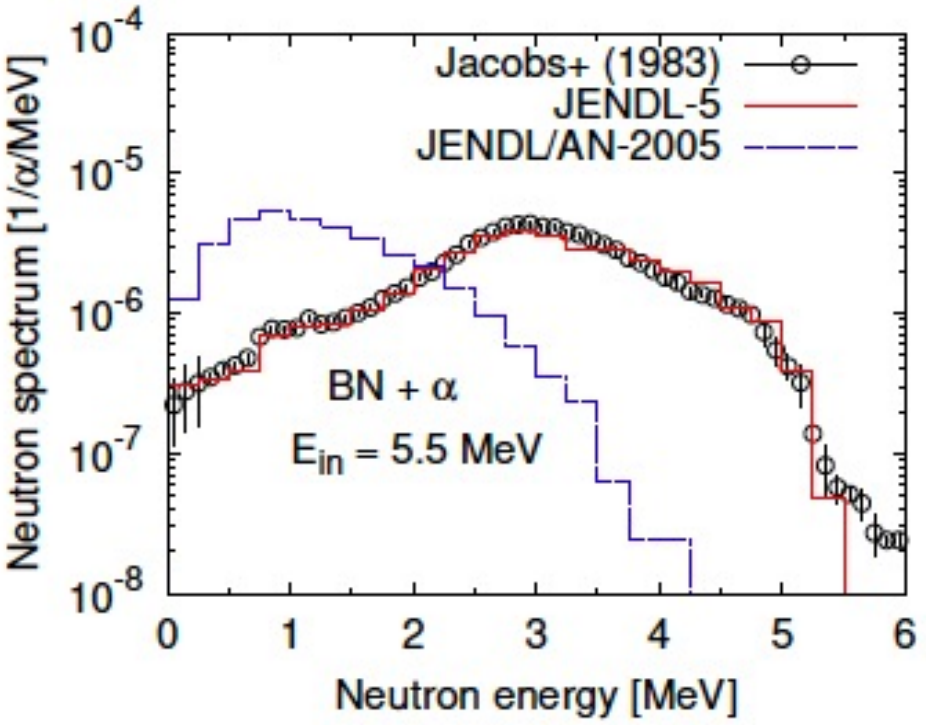
Q negative this time, but NJOY ismooth =1 ($\sqrt{E}$ shape) for when the evaluator decided to cut short the secondary energy grid of the recoil!

Challenges in representation

- (α,n_0), (α,n_1) and (α,n_2)
- Discreet peaks instead of continuous energy distributiom



No impact on n production but realistic spectra



Integrated values with respect to energy and angle are conserved in both cases

Challenges

- Enhanced completeness in evaluation
- Better physics to answers all foreseeable applications instead to only THE one
- Production of all γ-rays, charge particles and residuals nucleus state
- Issue with implicit evaluation, or above 20, 30 MeV ?

- Simulation
  - Converging heating may requires to converge multiple reaction rates at once
  - What exactly are the applications needs? Obviously they differ

Conclusions

- Evaluated is just a commencement, although it is seen as an end to an entire community
- 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
- NJOY plotr and viewr, PREPRO complot and evalplot are underrated verification tools
- FUDGE, ACEtk, ENDFftk will have to follow

Thank you for your attention!

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