Nuclear data structure and format: applications or science driven ?

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Preamble

- There seems to be a misconception or at least some degree of confusion within the nuclear data communities at large so as what type of information are, can, should or cannot be extracted, processed for any particular applications out of an evaluated file ENDF-6's formatted.

- The degree, accuracy, completeness of the processed data streams strongly depend on, is influenced by the evaluated file format frame and the processing protocols available.

- Particular application needs usually dictate the processing protocols to be implemented.

Evaluated file format

- Experience based on ENDF/B, JEFF, JENDL, TENDL, EAF formatted files
- Since the dawn of the nuclear age the dogmatism of few nuclear technology (# sciences) applications has shaped the format frame of each and every evaluated file/library
- This was carried on, shaped through the many corrections and clarifications of what has become the ENDF-6 format manual

- S10/20/30 MeV file format (s20 switch, transition energy)
- S0 file format
- Activation-transmutation file format
- Dosimetry file format
- …

Now a day the fits are tights

Evaluated file format

- S0 formatted file: every things in one single mf-3/mt-5*mf6 (works for simple transport, shielding, high-energy physics)

- S30 formatted file: mf-3/4/5/6+ detailed up to 30 MeV, then as above from 30-200 MeV (works, needed for criticality, safety, shielding, low energy physics)

- Activation-transmutation formatted files: partials, total cross-sections to all stable and radioactive (decaying) residuals and emitted (A<4) particles and spectra (needed for activation-transmutation-source terms and material sciences, low and high energy physics)

TENDL files

Each isotope in TENDL comes in 7 different structures:

- S0: no explicit MT numbers, only MF3/6-MT-2,5,18
- S20: explicit MT's < 20 MeV, g in MF12, MF32; MF3/6-MT-2,5,18 > 20 MeV (original extension of ENDF/B (LA-150))
- S30: explicit MT's < 30 MeV, g in MF-6; MF3/6-MT-2,5,18 > 30 MeV ("THE" standard TENDL file, for the standard distribution)
- S60: explicit MT numbers below 60 MeV, MF3/6-MT-2,5,18 above 60 MeV (used by the old FISPACT, for plotting purposes)
- MT: explicit MT numbers up to 200 MeV and gradual "ingrow" of MT5 after a few tens of MeV (EMPIRE-based evaluations, Trkov-style)
- ACF: ENDF-formatted activation file
- EAF: EAF-formatted activation file

Libraries format frame

- TENDL-2017 contrasts with the major libraries: ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0 or CENDL-3.1 in two ways of some importance

  1. All targets are delivered in an identical format frame

  2. Seven format frames co-exists

- For all the other libraries, the format frame of each and every targets depend more on when it was evaluated, by whom, for which application, etc.. This inevitably lead to processing and derived data uniformity and quality issues

File releases

Each major library project has its own naming convention for isotopic data files:

e.g.: n-26-Fe-56.jeff32, 26-Fe-56g.jeff33, n-026_Fe_056.endf, Fe056.dat, n-Fe056.tendl, Fe056, etc..

One policy can be agreed upon, suing well-defined protare’s

n-Fe056.jeff3.3

n-Fe056.endfb8.0

n-Fe056.irdff2.0

…..

n-Am242m.tendl.2017

Evaluated file format

- There is a need now a day to better serves nuclear sciences to have a deeper interpretation of the experimental landscape
- There is a need to properly correlate nuclear observables, go deeper, further in the nuclear scales
- There is a need to find better foundations to allow the physic models to goes where no measurements can or will
- There is a need for evaluated file to be complete but also reliable, trustworthy outside their standard V&V framework
- There is a need for all applications data to stem from a single unique container

Nuclear reaction and data modelling

- There are some factors that can influence the outcome:
  - Incident particles: neutral, massless or charged
  - Incident energy range: low and/or high
  - Nuclear models choice
  - With or without the influence of nuclear experiments and observables data
  - Evaluation techniques: hand-crafted and/or automatized
  - For nuclear technology and/or nuclear science
  - For a publication and/or an application
  - For general/single/multi-purposes
  - …

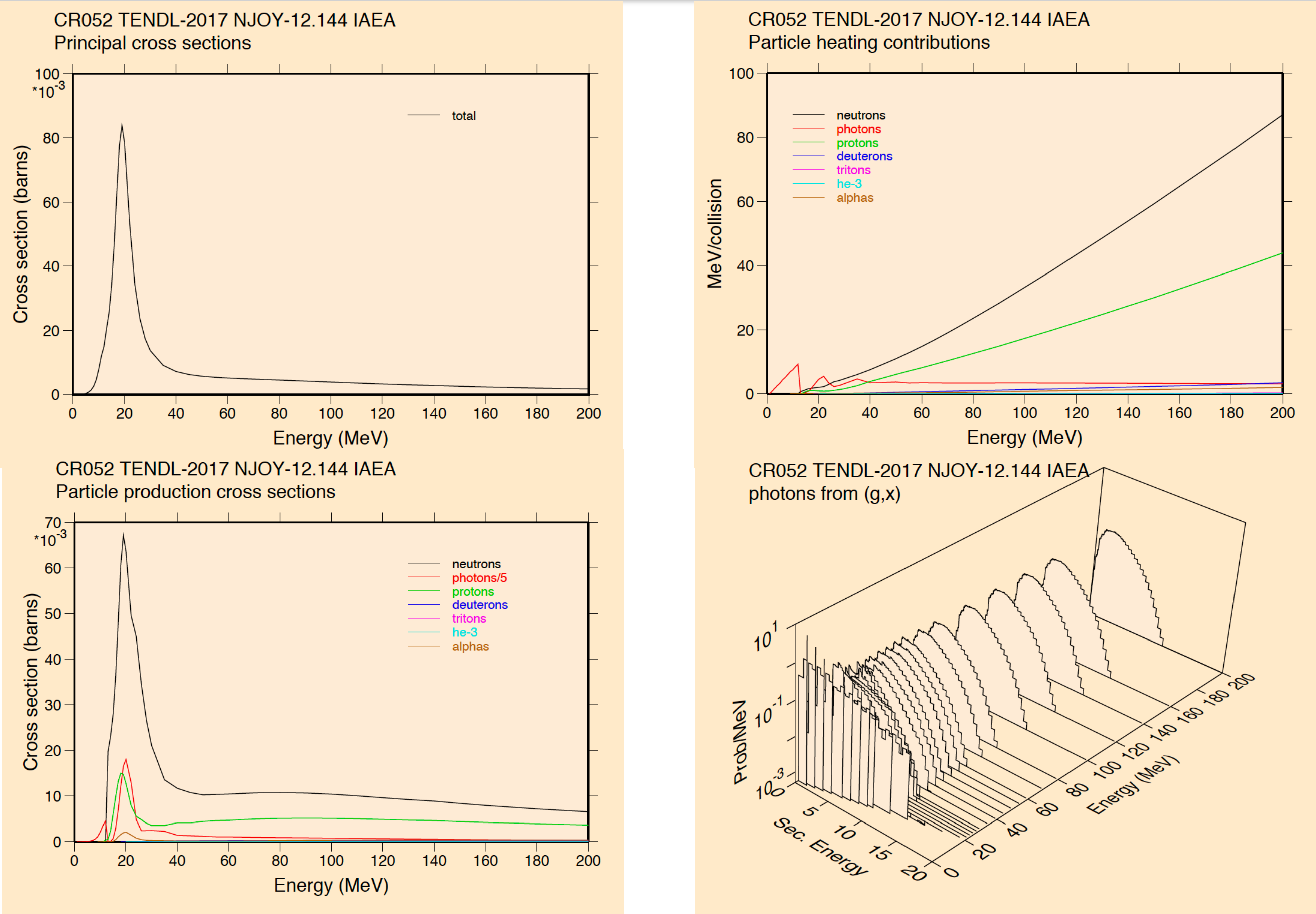
Nuclear reaction and data modelling

- A lot boils down to two concepts: exclusive or inclusive

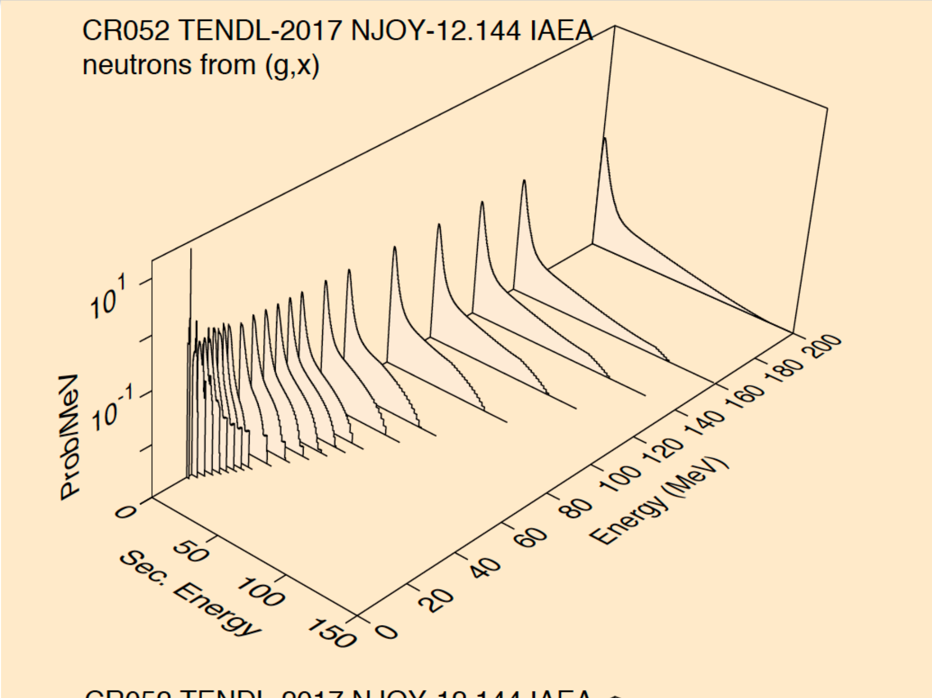
- A reaction is defined as exclusive when the outgoing channels are precisely and uniquely specified by the type and number of outgoing particles and any number of photons. Usually, all exclusive reactions sum-up to the non-elastic. This tends to lead to S30 type file format

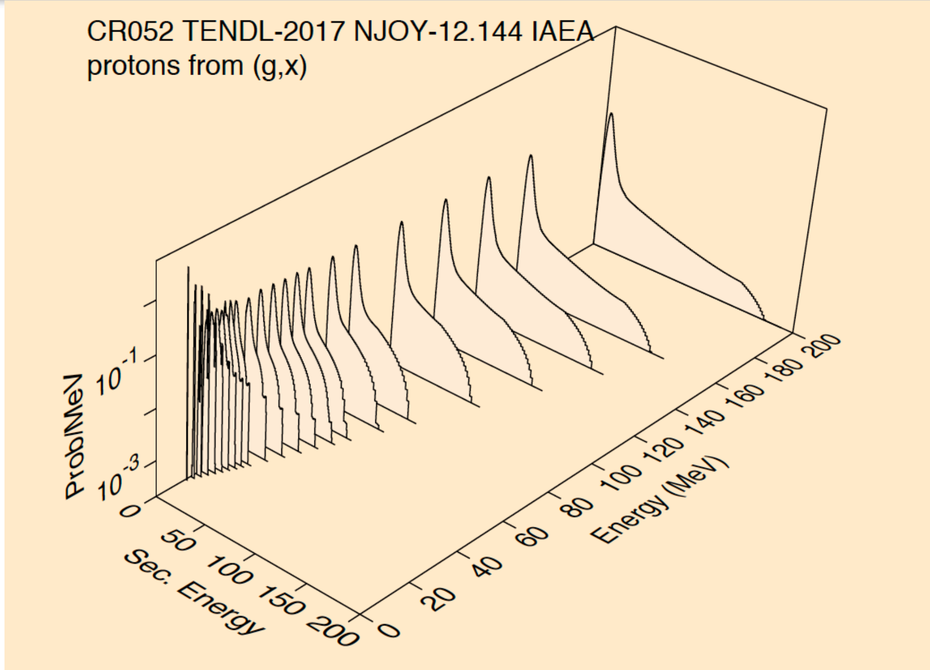
- For typically more than 4 ejectiles, an open channel inclusive reaction per excitation energy model is preferred, that allow to track particles (A<4) and residuals production cross section. This tends to lead to S0 type file format

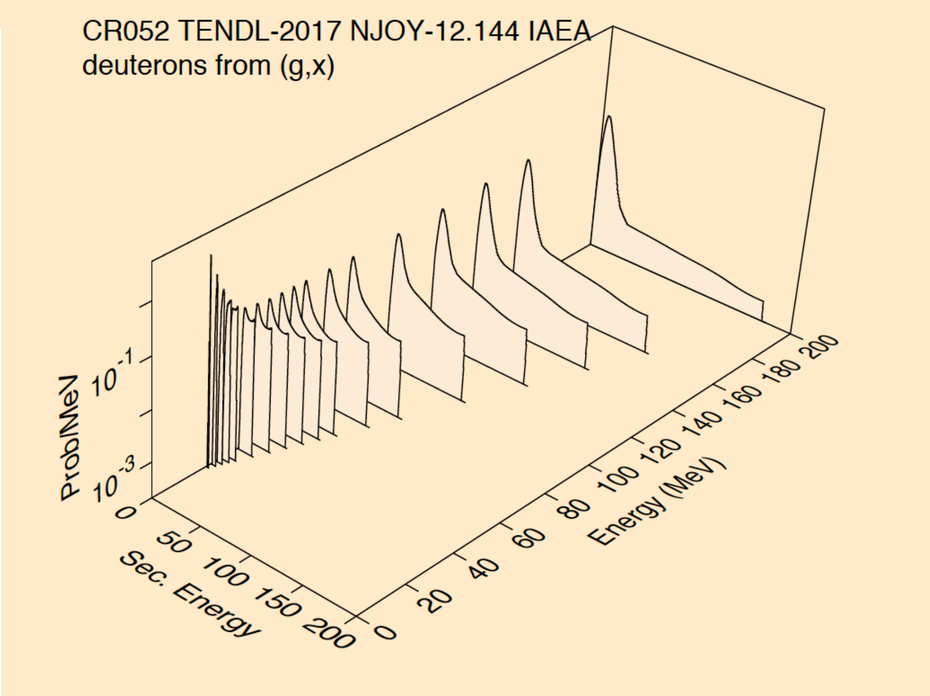
Application library: transport from an S0

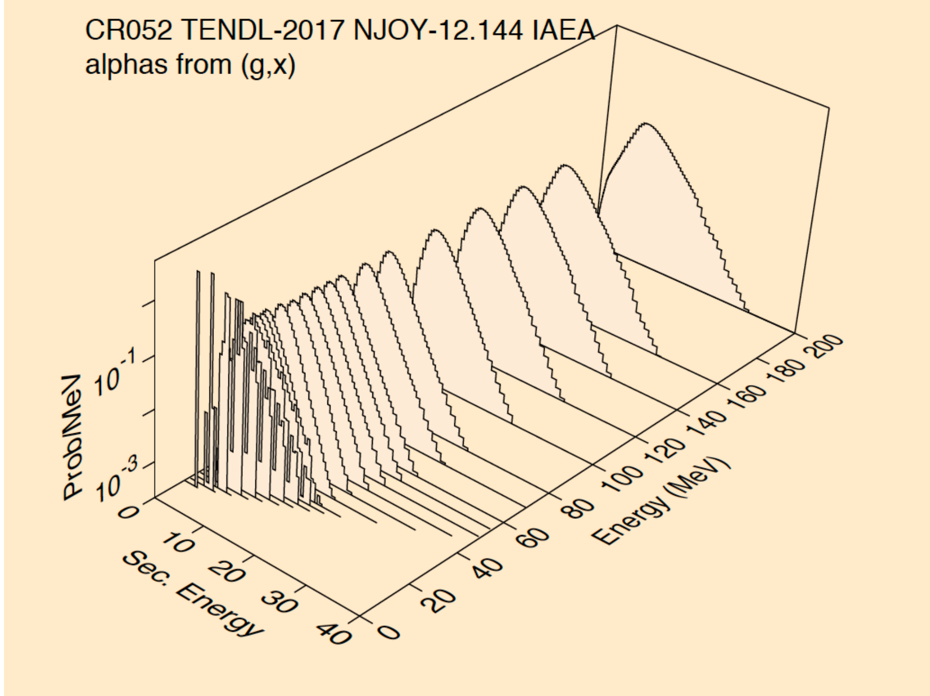


Application library: transport from an S0

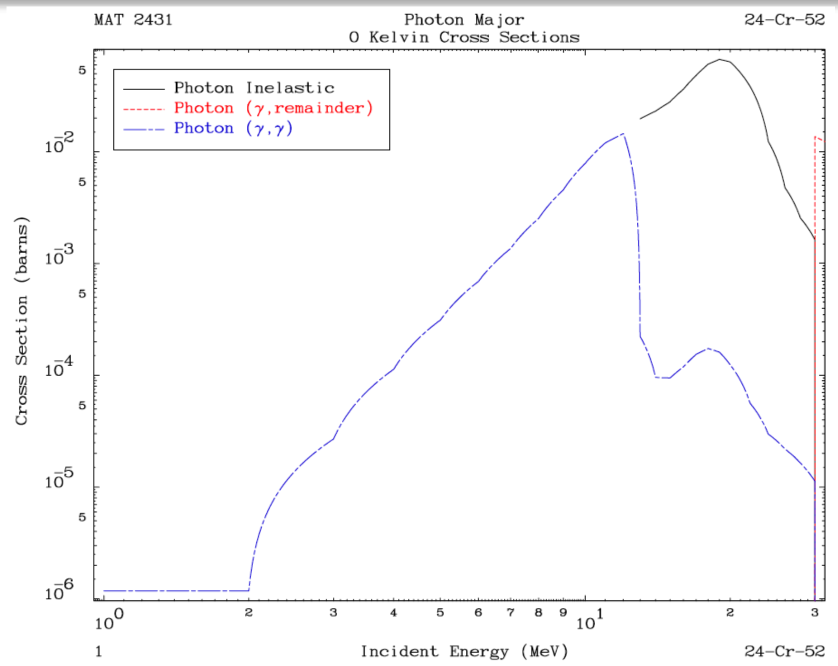


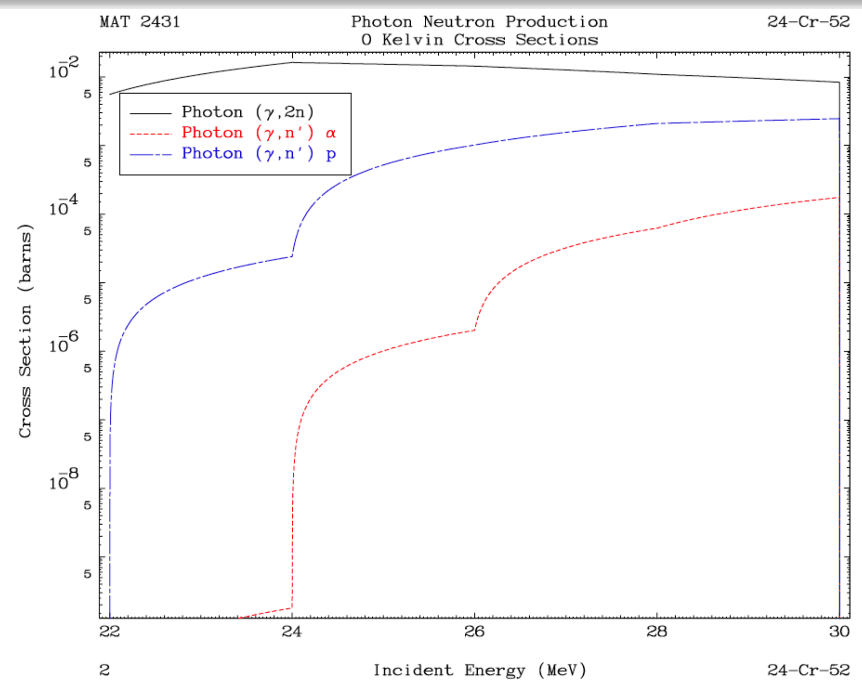


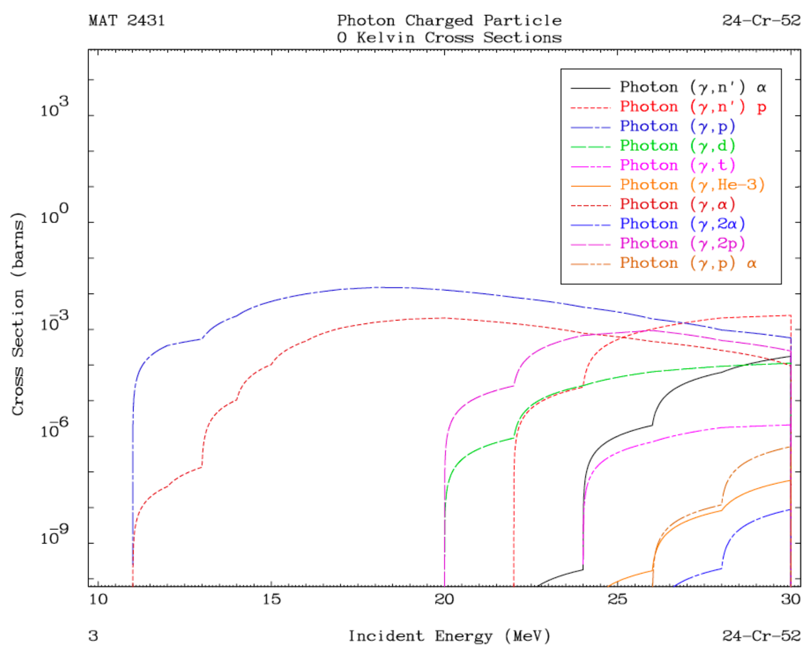


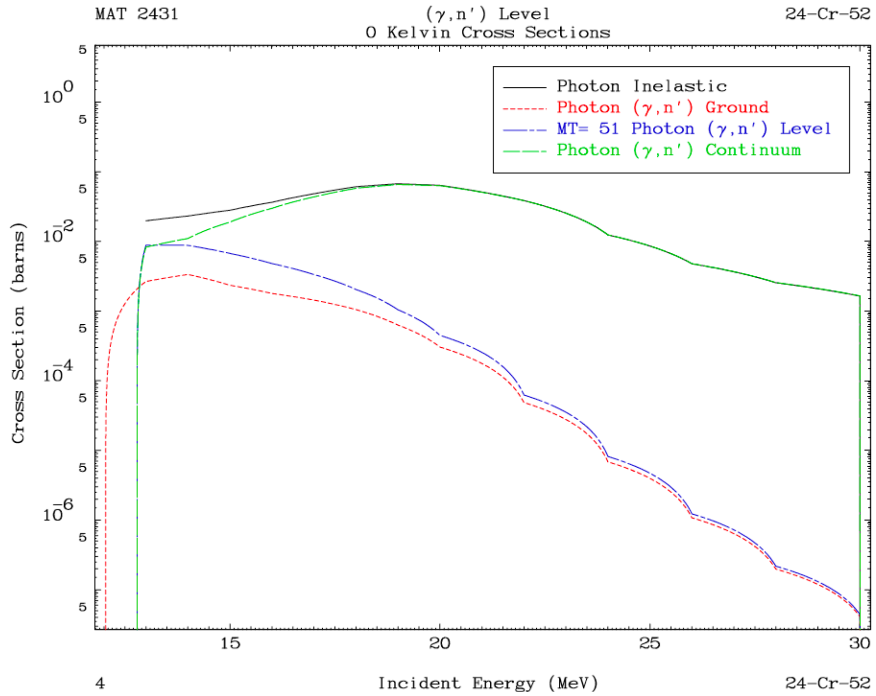


Application library: detailed MT's from a S30

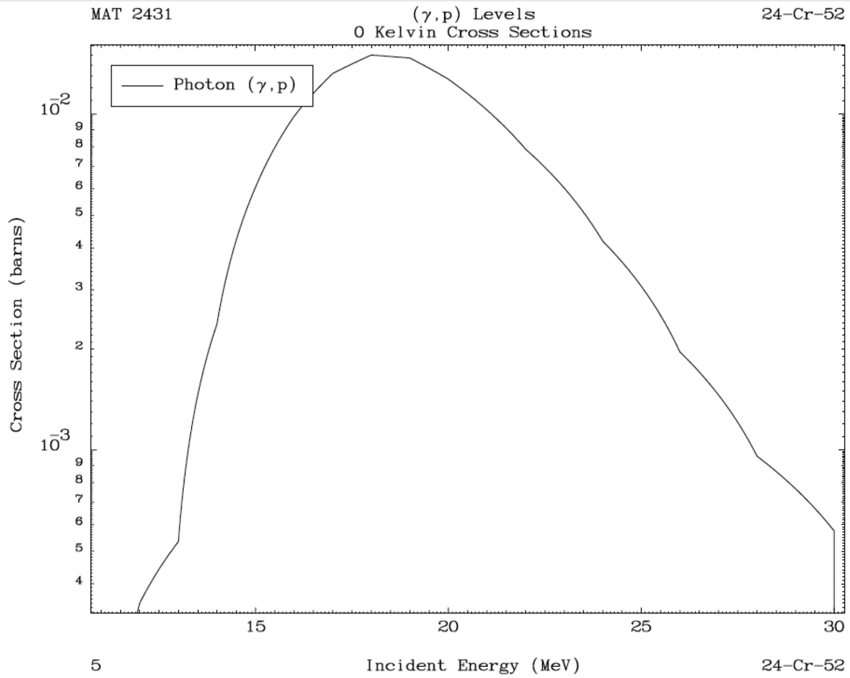


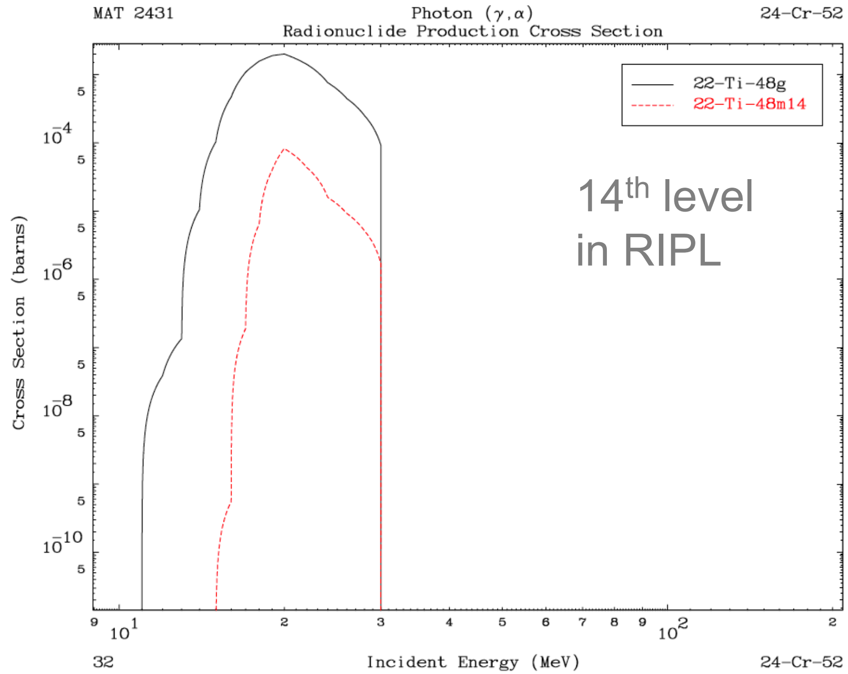


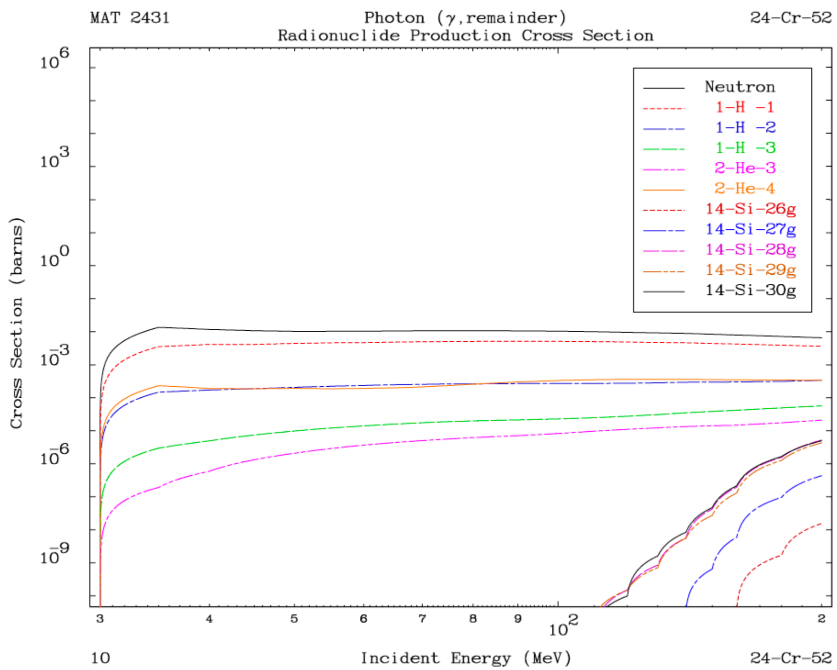


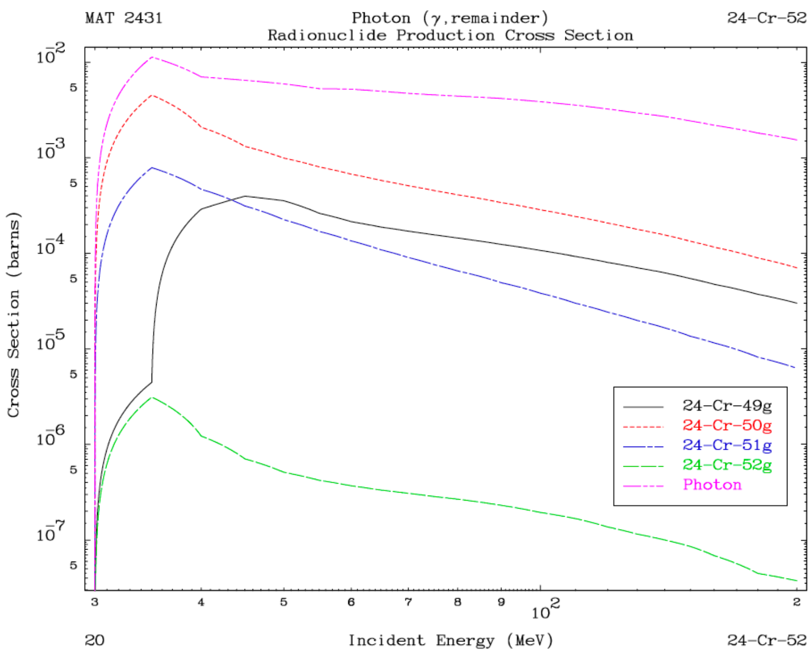


Application library: detailed MT's from a S30









What's matter

- Data container (prompt)
  - Uniquely defined cross section channels data, total and partials
  - Emitted particle types, energy-angle distribution
  - Excited, isomeric states residual data
  - Isomeric branching ratio

  And this across all the incident particle energy space

- Derived data
  - Constrained T-dependent pointwise-groupwise/angular/spectral data with clear sum-up rules
  - Heating-Dose: energy balance and/or kinematic
  - Gas production

- Delayed, decay metrics

What's matter

- ^{60}Ni (n,g) ^{61}Ni = activation channels
- ^{60}Ni (n,2n) ^{59}Ni = activation channels
- ^{60}Ni (n,t) or (n,nd) ^{58g,58m}Co = four partials transmutation channels
- ^{59}Ni (n,p) ^{59}Co = transmutation channel
- ^{60}Ni (n,np) or (n,d) ^{59}Co = two transmutation channels
- ^{60}Ni (n,a) ^{57}Fe = transmutation channel

- ^{235}U (n,f); (n,g); (n,a) = absorption, burnup channels
- ^{238}U (n,g) ^{239}U= absorption, activation, enrichment channel
- ^{238}U (n,n') = total inelastic scattering, leakage channel

- In reactor physics if you only need to assess the neutron spectra or map, the residual, non neutron emitted particles matter little.

Data container

- Ambiguity on:
  - Excited and/or isomeric state definition
  - Incident energy grid reconstruction criterion
  - Residual state definition
  - Complex emission metrics: fission (υ,P(υ),FF(υ),..) but also compound/direct/continuum and breakup events. Where the data or the observable needed is in fact derived, assembled from more basic physics information

- The state of all predicted residuals need to be uniquely defined in the file: ZAP Elevel (# integer or letter)
- The multi-scale,-step aspect of the physics at play need to be respected

Data container

- Event generator provides correlated particles and photon emission
  - The energy and momentum of the sampled particles are conserved for each event, as opposed to ENDF-6 typical energy/angular spectrum representation

This is particularly important for in depth study of detector responses, such as for:

  - Measurements in coincidence
  - Material sciences
  - Micro dosimetry

- Monte Carlo simulation would take advantage of the full capability of Hauser-Feshbach (CGMF, FREYA, ..) fission event generator

Conclusions

- The structure of the data need to better follow the physics, instead of a single particular application need
- All pre and processing protocols need to be clearly established, identified and exemplified
- A container structure could have more than one representation of observables:
  - Resonance parameters and reconstructed channels
  - Total and partials cross section, on a unique grid
  - Self-shielding factors (in the URR)
  - Total and component data
  - ….
- Physic (Astro-, Plasma-, Nuclear-, Medical-,..) sciences driven format frame prior to an ENDF-6 format