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Multifaceted coded nuclear data libraries assemblage: TENDL-2023

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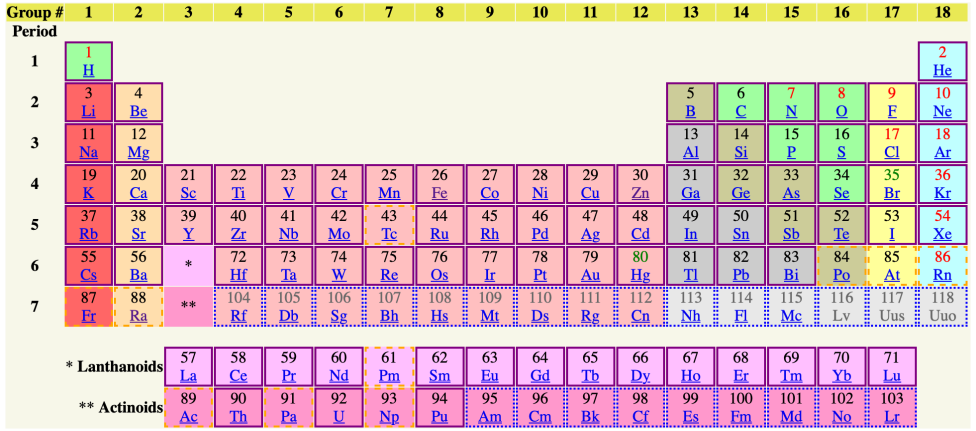
Dr. Eng. IAEA Unit Head

The making of TENDL-2023 – repeatability and innovation

- 7 incident particles: alpha, gamma, deuteron, proton, helium, triton and neutron induced libraries
- 2813 targets Z=1-115, Hydrogen to Moscovium, including as target some 513 m (1st), 30 n (2nd) isomeric states (T½ > 1s)
- TENDL describes all open reaction channels, product yields, emitted spectra, and short-lived daughter radionuclides (T½ > 0.1s) up to 200 MeV, with covariance derived from reference input parameters variation
- 12th version



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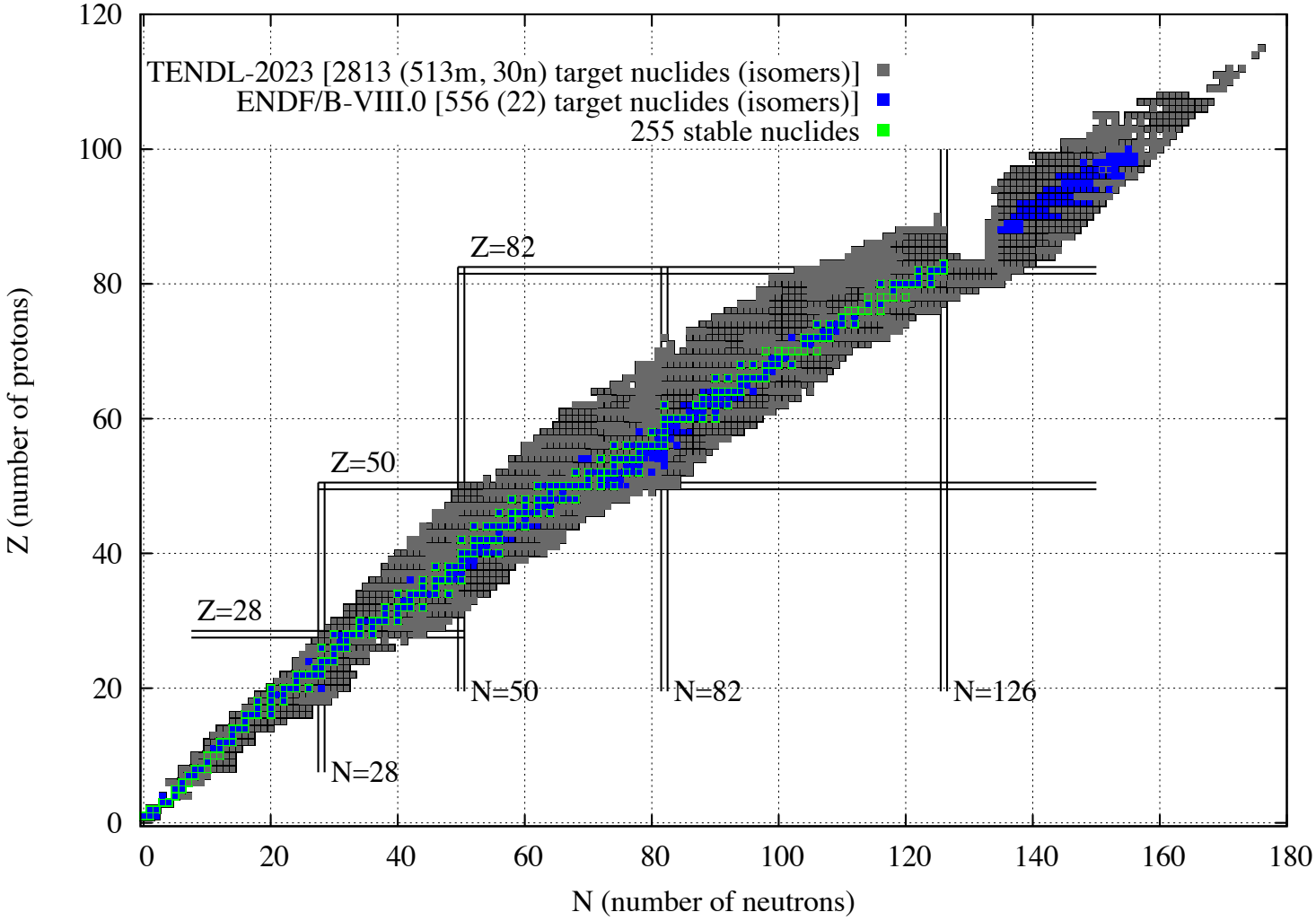
Nuclear landscape: Isotopic targets

Incident

-neutron
-gamma
-proton
-deuteron
-triton
-alpha
-helion



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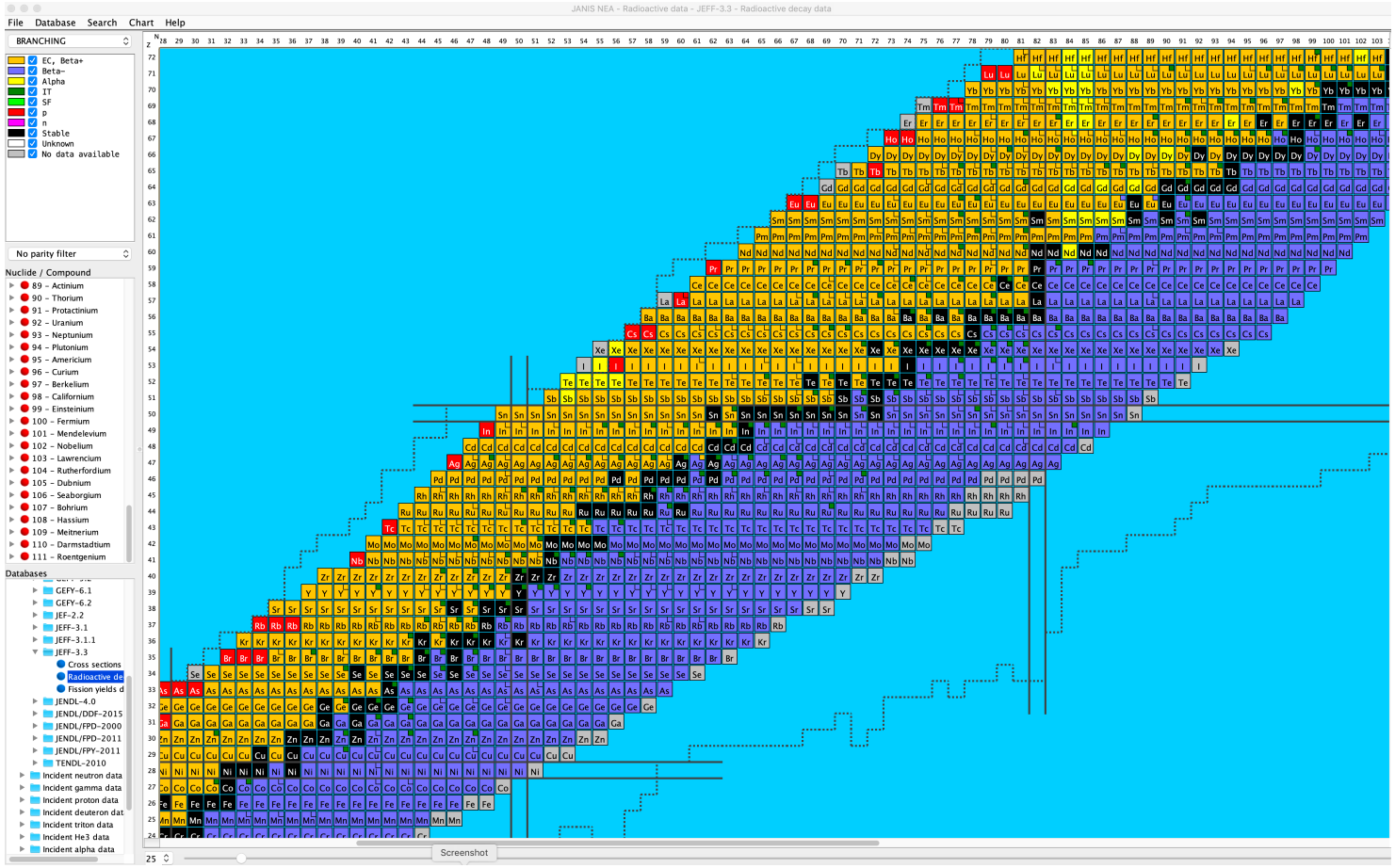
Nuclear landscape: Isotopic residuals & decays

- Radioactive decay data: 4035 “reaction daughters” or “residuals”



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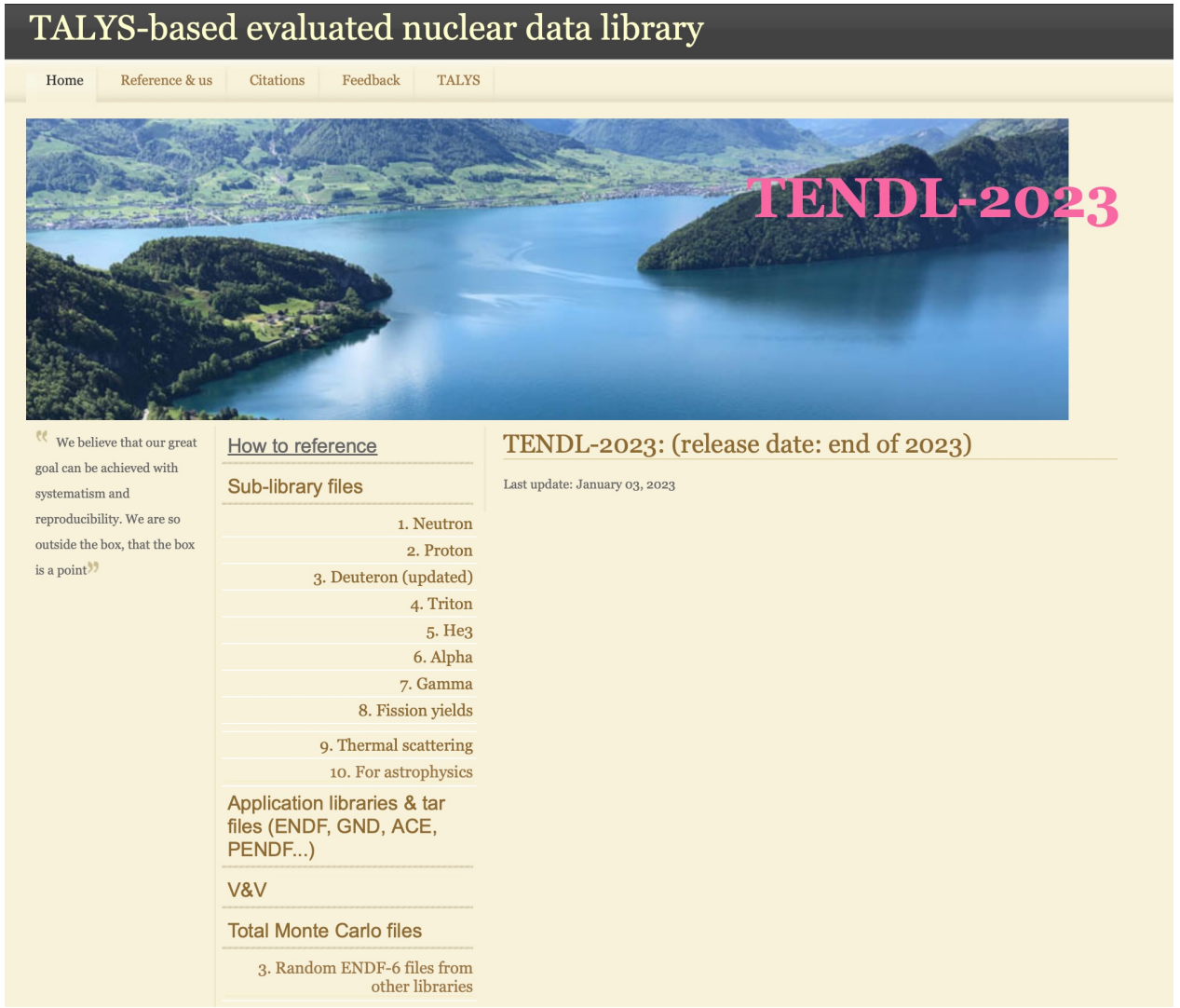
Portal https://tendl.web.psi.ch/tendl_2023/tendl2023.html

- Tabular forms
- ENDF-6: explicit s30 and implicit s0
- GNDS explicit
- Variance-Covariance from model parameters
- Plots, films
- …



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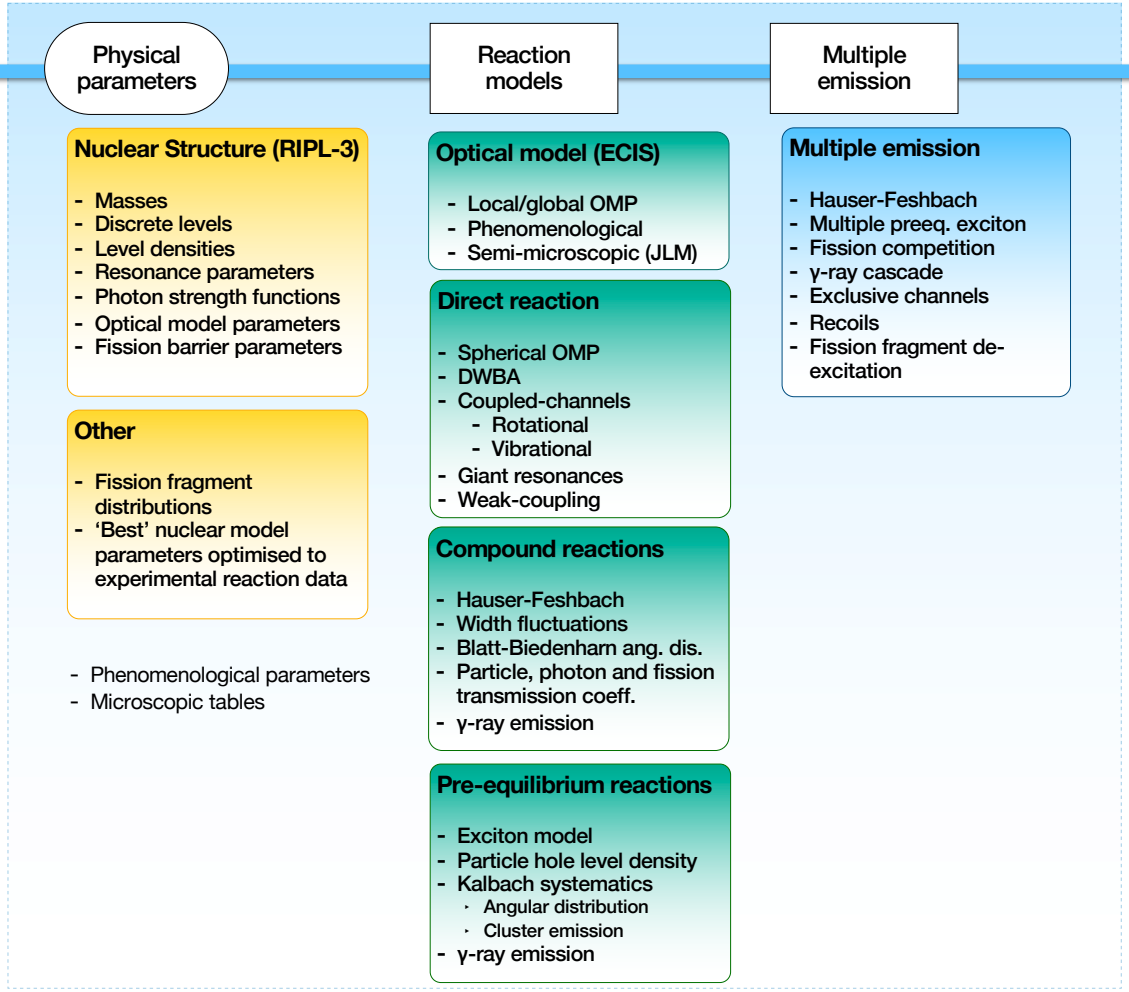
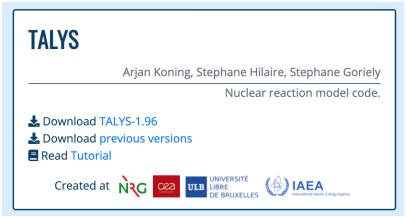
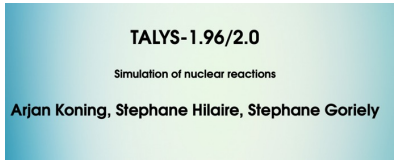
TALYS 1.96 https://tendl.web.psi.ch/tendl_2021/talys.html




```
projectile n
element Fe
mass 56
energy 14.0
```

+ some 400 keywords





Output files per reaction channel

- Cross sections
  - Total
  - Exclusive: (n,γ), (n,f), (n,n'), (n,2n), (n,p) etc.
  - Per level
  - Residual production
  - Particle production
  - γ-ray production
- Emission spectra
  - Single-differential
  - Double differential
  - Recoils
- Angular distributions
  - Elastic
  - Per level
- Particle multiplicities
- Fission yields, neutron observables
- Astrophysical reaction rates, MACS
- …

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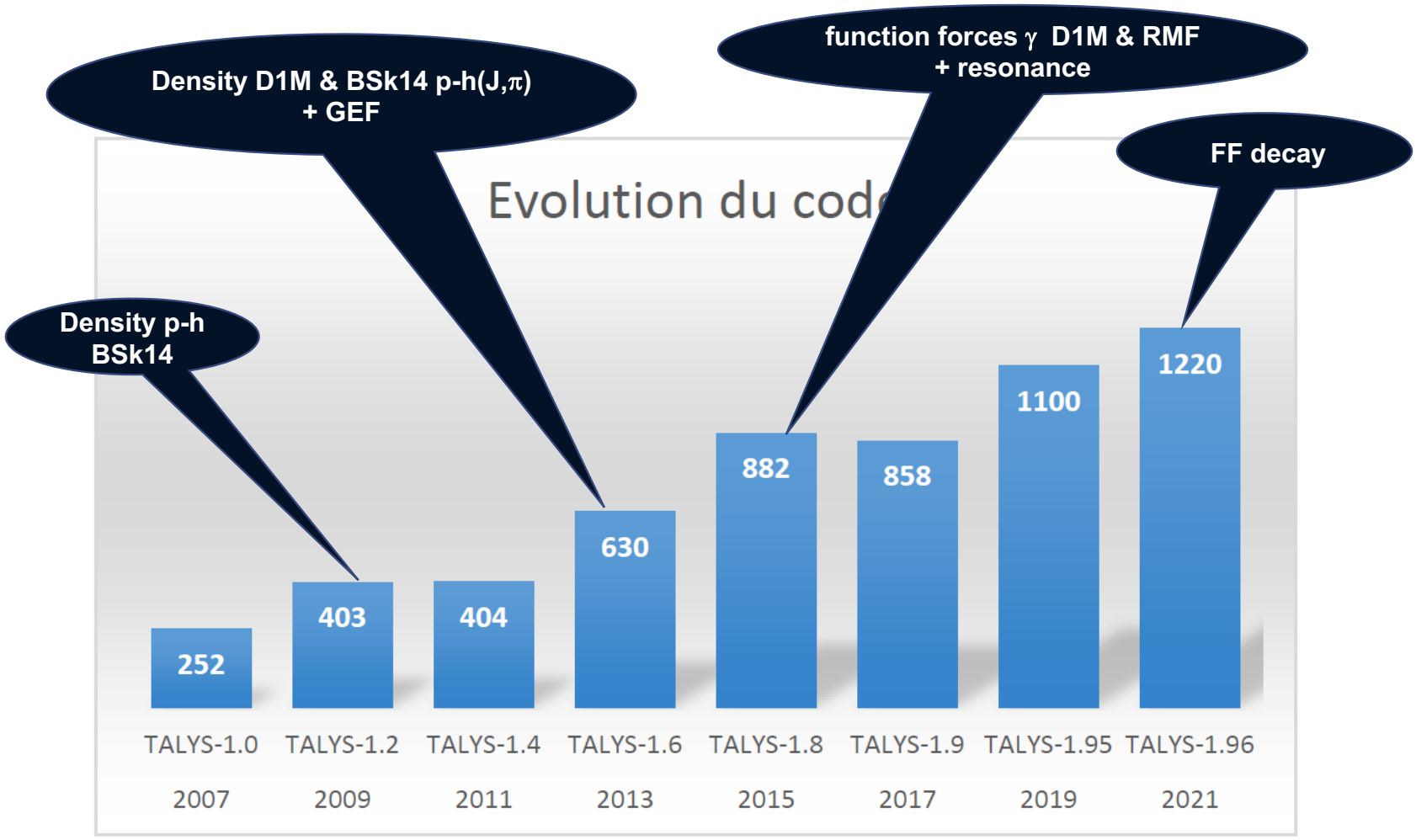
TALYS time steps evolution



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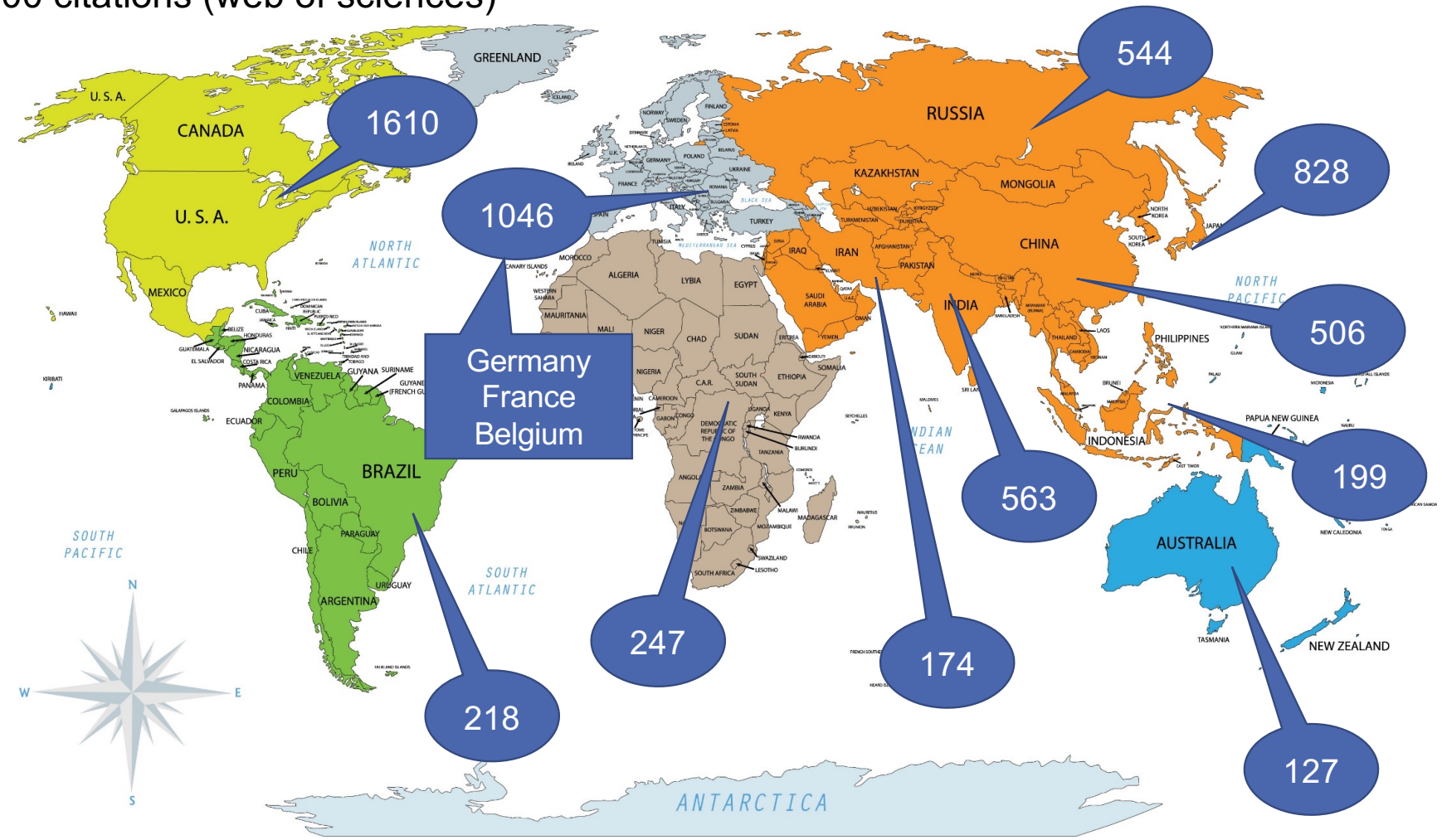
TALYS around the World

- Around 5500 citations (web of sciences)



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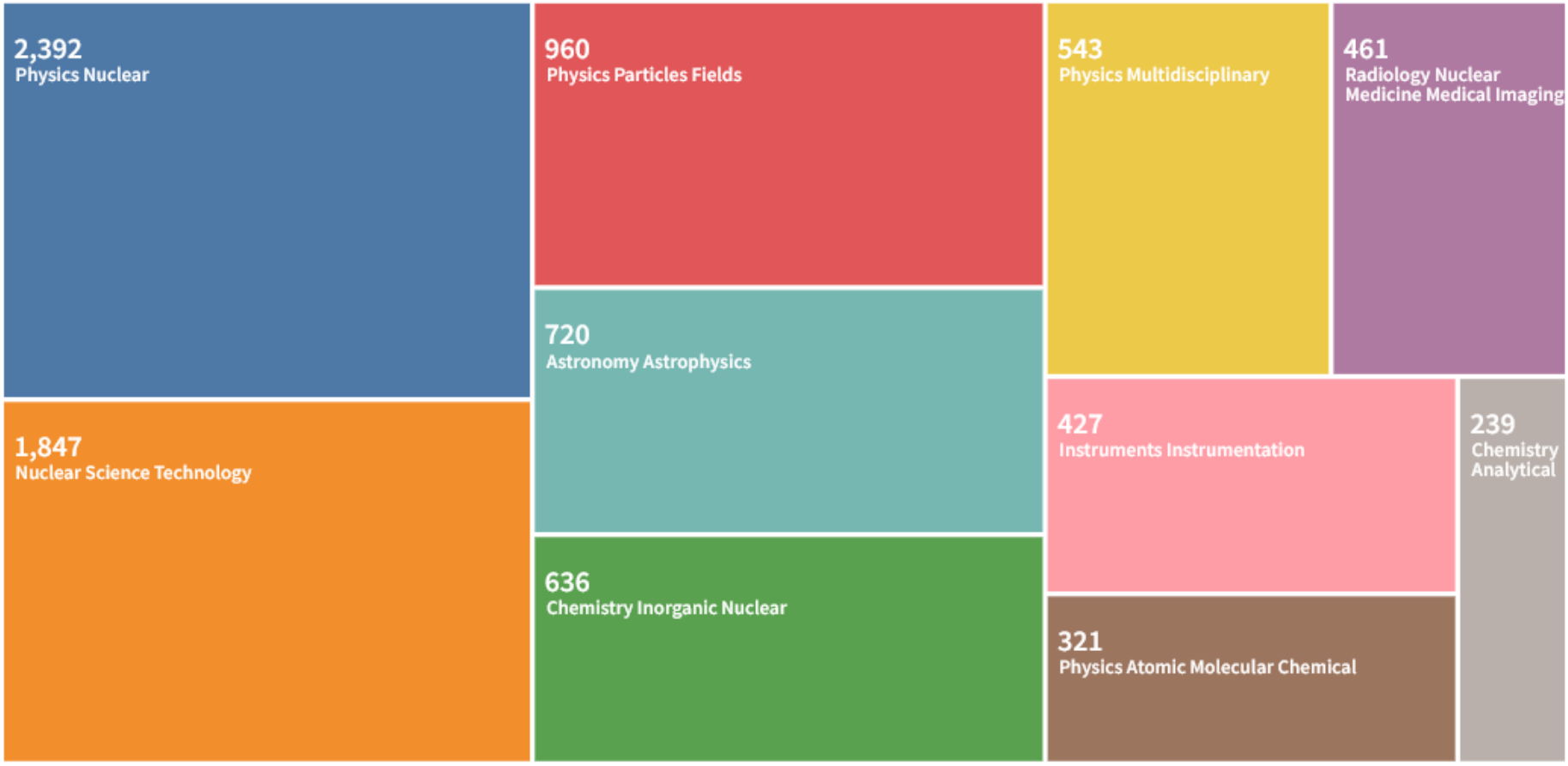
TALYS applications in the World

- Around 5500 citations (web of sciences)



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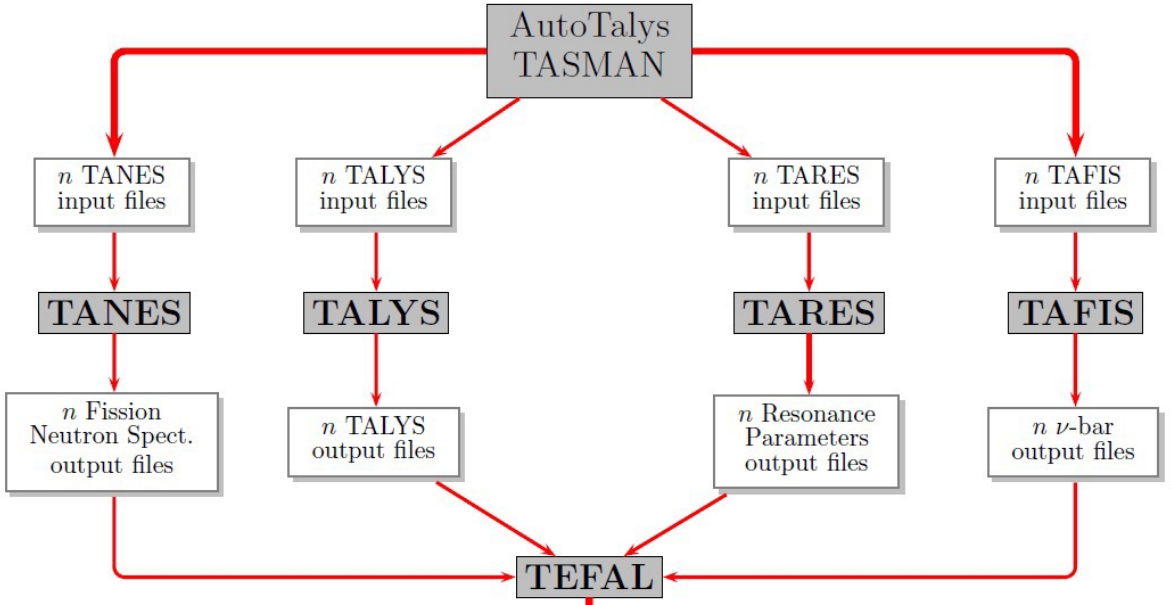
T6: automatisation – reproducibility - robustness

- TALYS, TANES, TARES, TAFIS, TEFAL, TASMAN



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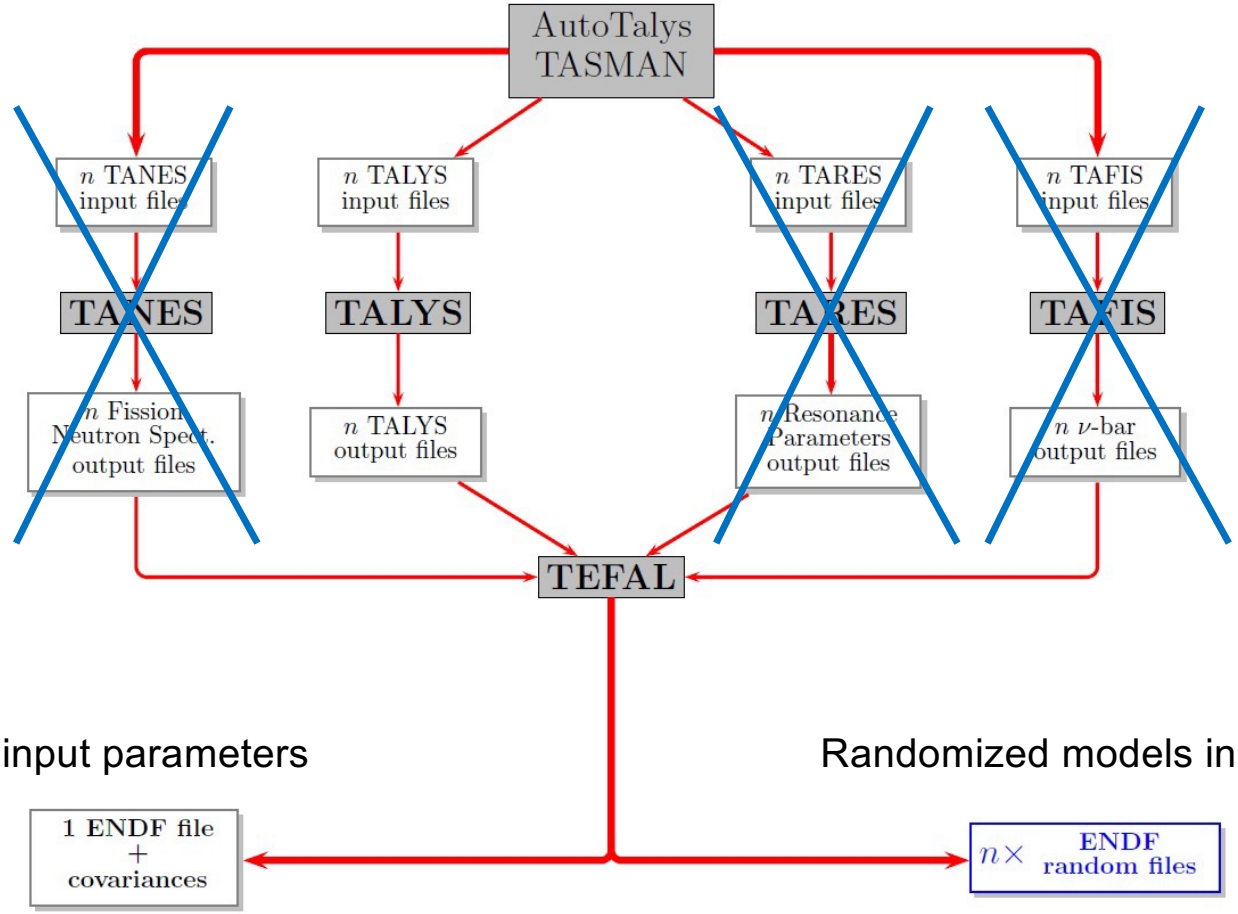
T3: automatisation – reproducibility – robustness - simplification

- TALYS, TEFAL, TASMAN: version 2.0



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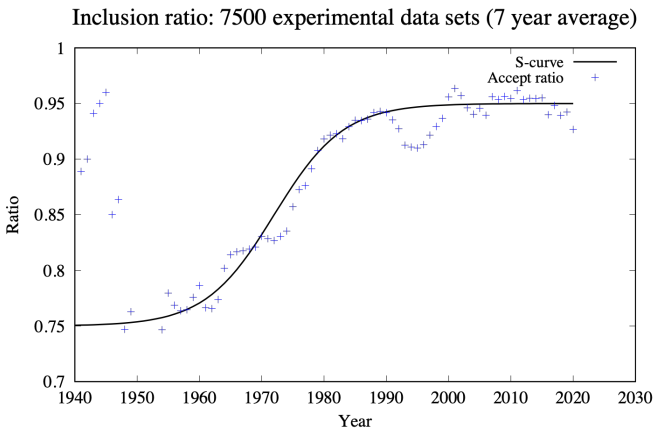
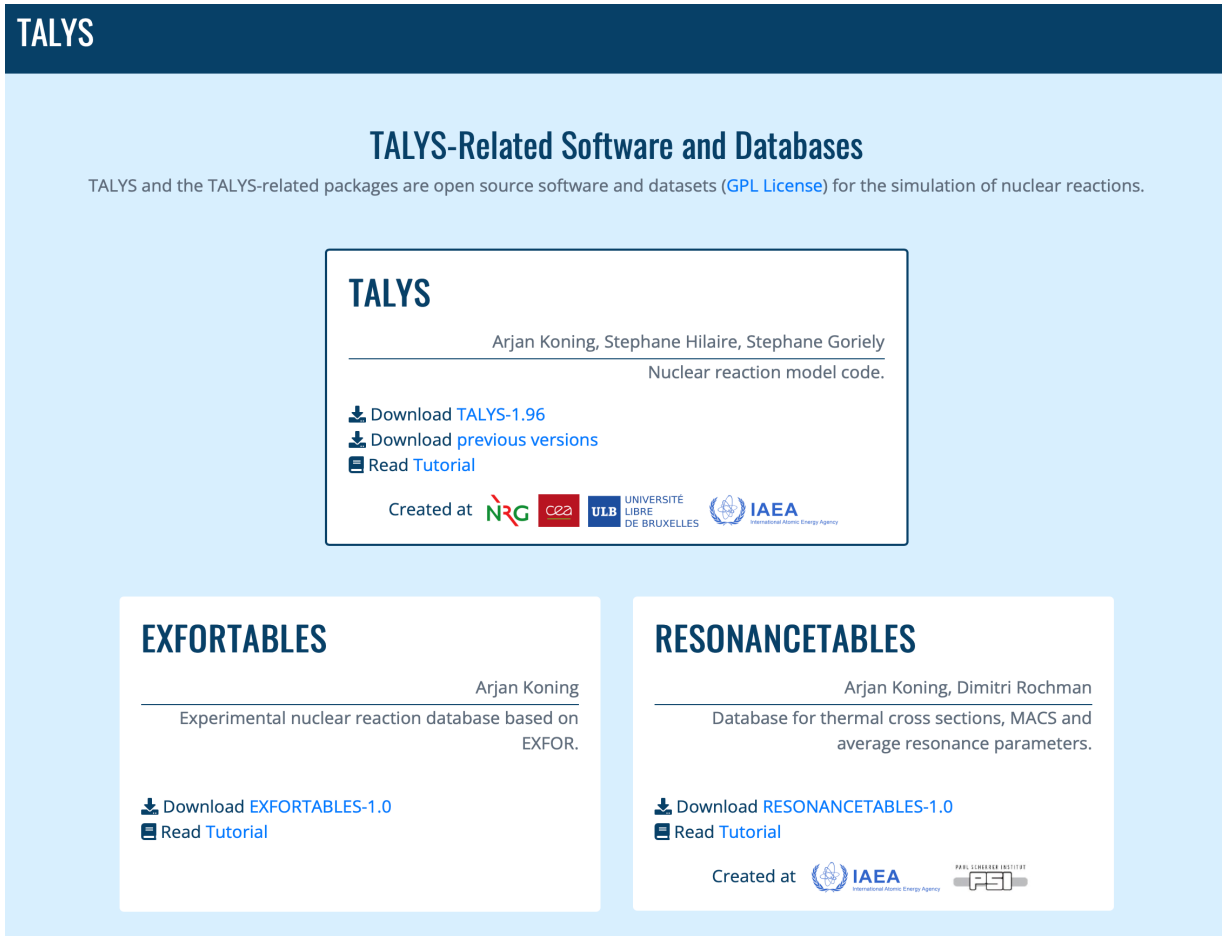
T3: TALYS, TEFAL, TASMAM + resbase

- RESONANCETABLES ready to use resonance parameters

https://www-nds.iaea.org/talys/

7500 experiments, age weighted, subjective, but..





For all 2813 n-targets

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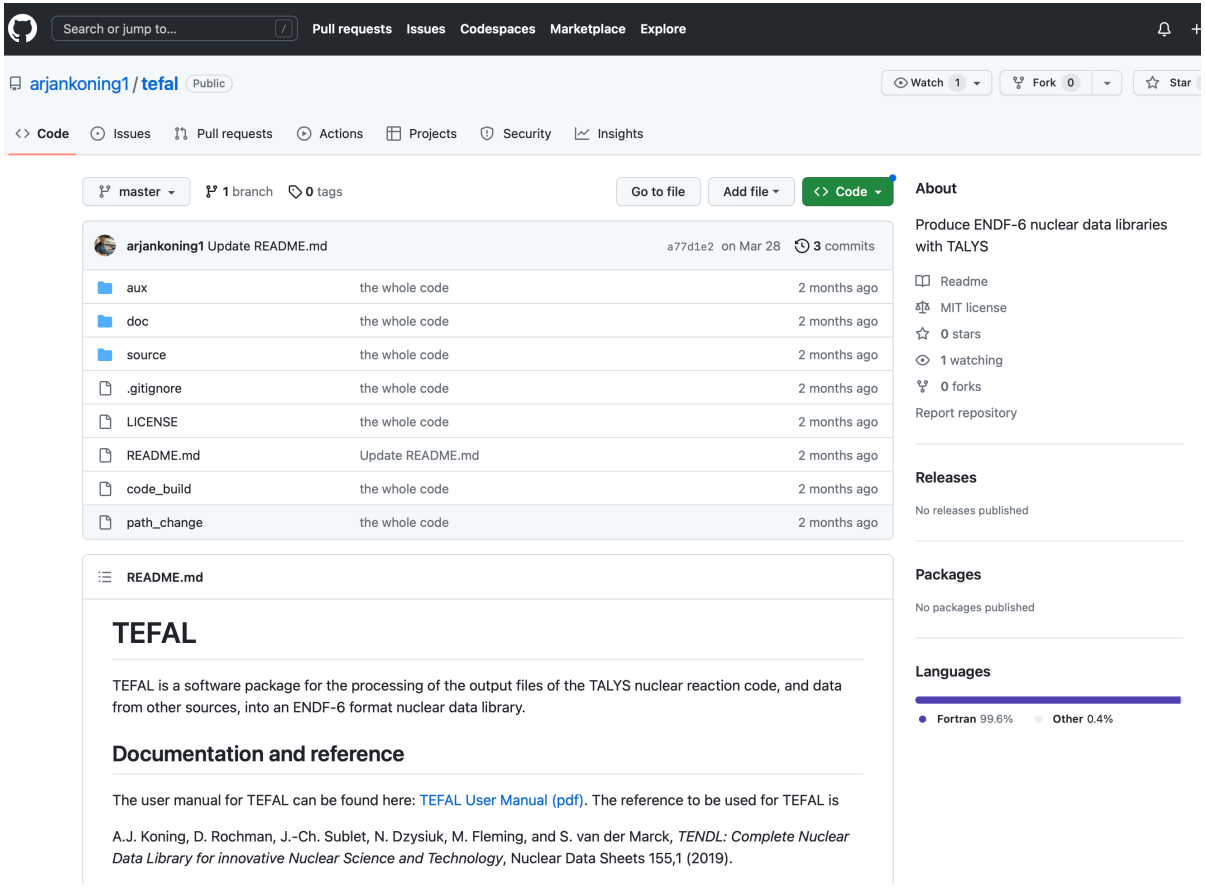
T3: TALYS, TEFAL, TASMAN + resbase

- Distribution: Github https://github.com/arjankoning1/tefal
- TEFAL

Also aiming for

- TALYS
- TASMAN



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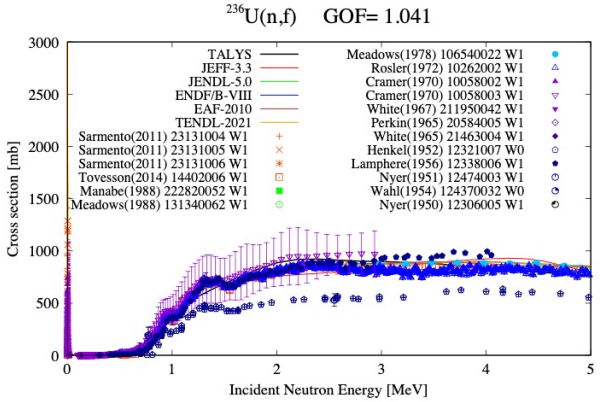
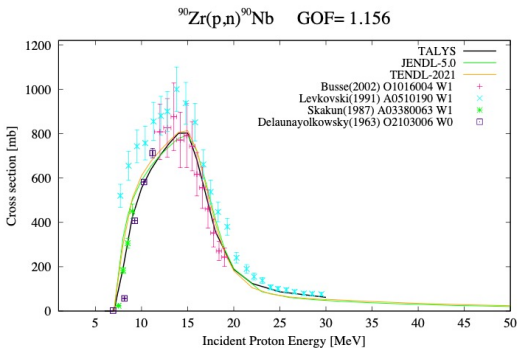
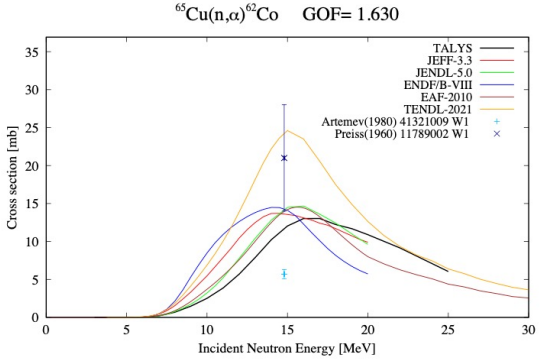
TALYS coded input parameters & GOF

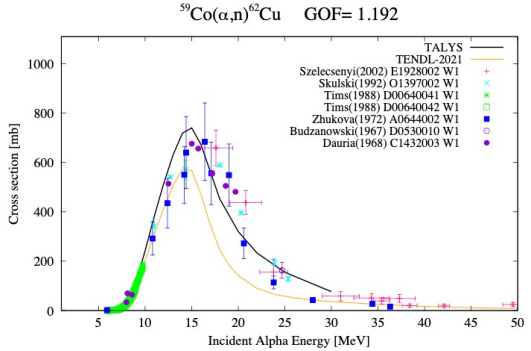
- Optimized parameters
- Weight allocation on exp.

Reaction	Nuclides						
(n,γ)	278	wtable					
(n,f)	34	vfiscor	betafiscor	ctable(1)	ptable(1)	ctable(2)	ptable(2)
(n,n';2n;p)	210	rv(p)	$g_{ph}(0)$	$g_{ph}(n)$	ctable(n)	ctable(p)	
(n,α)	157	rv(α)	Cstrip(α)	$g_{ph}(0)$	ctable(α)		
(p,n)	142	rv(p)	rwd(p)	rv(n)	$g_{ph}(0)$	$g_{ph}(n)$	ctable(n)
(γ,n)	77	wtable	ftable	etable			
(α,n)	93	rv(α)	rwd(α)	rv(n)	$g_{ph}(0)$	ctable(α)	
(d,n)	40	rv(p)	rwd(p)	rv(n)	$g_{ph}(0)$	$g_{ph}(n)$	ctable(n)









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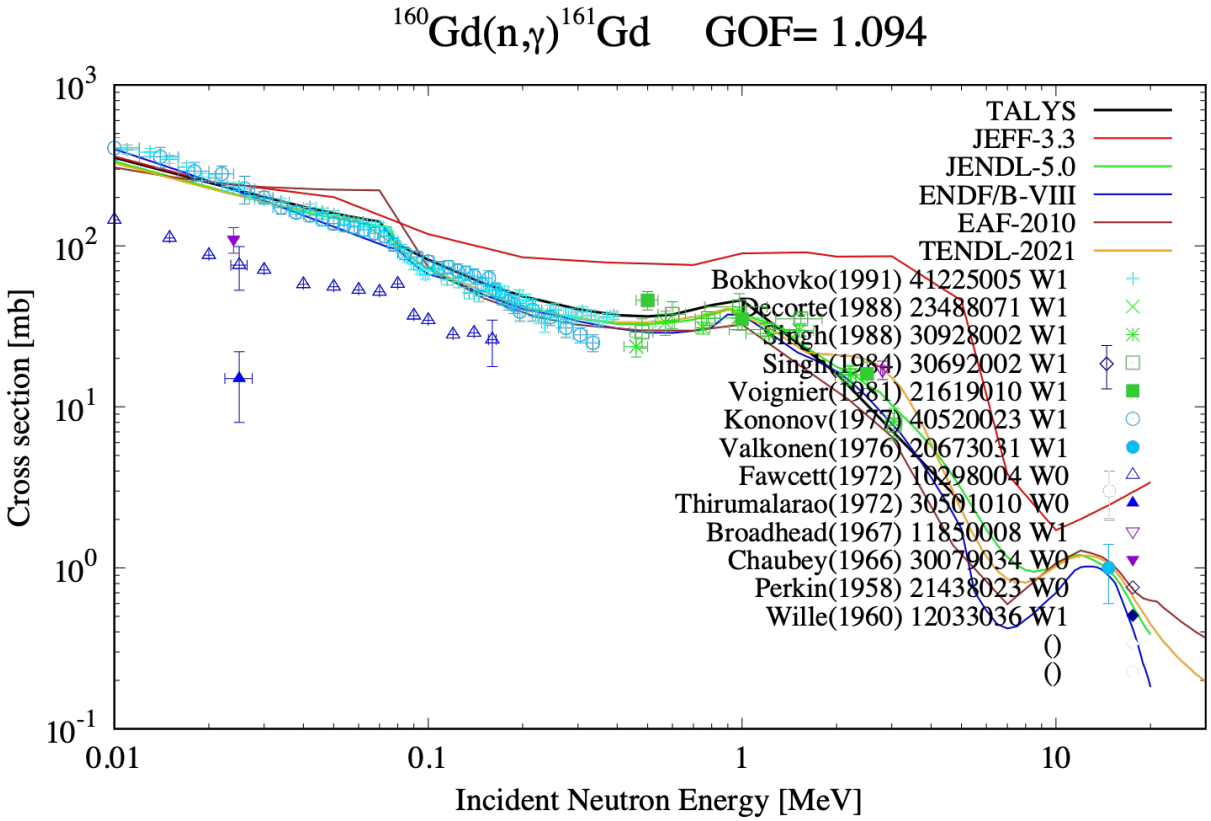
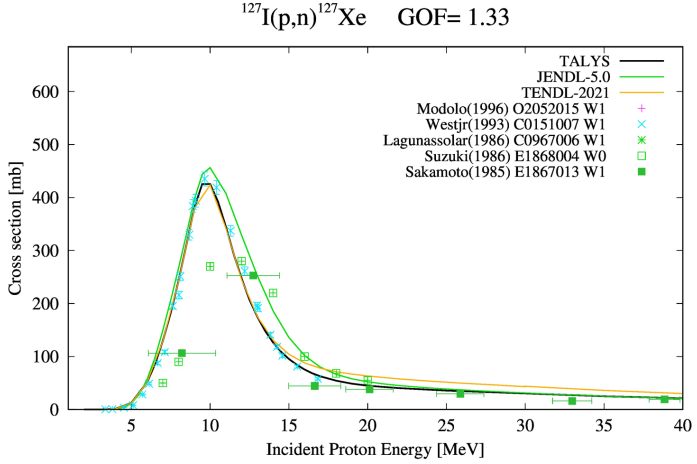
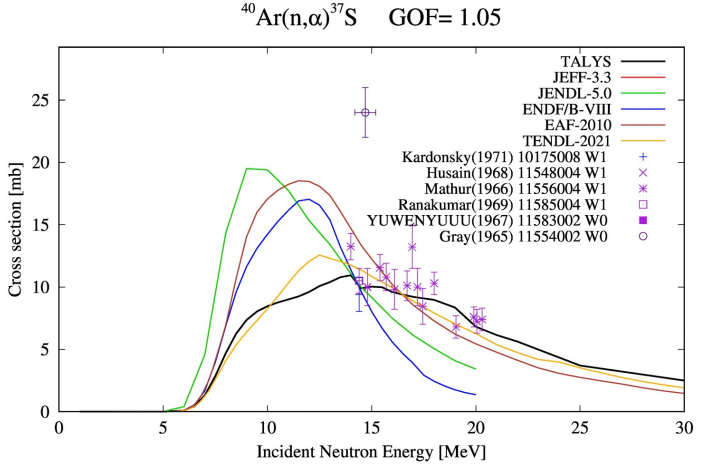
TALYS coded input parameters & GOF

- Outlier assignment (W0) and optimised TALYS model parameters per nuclide and reaction channel

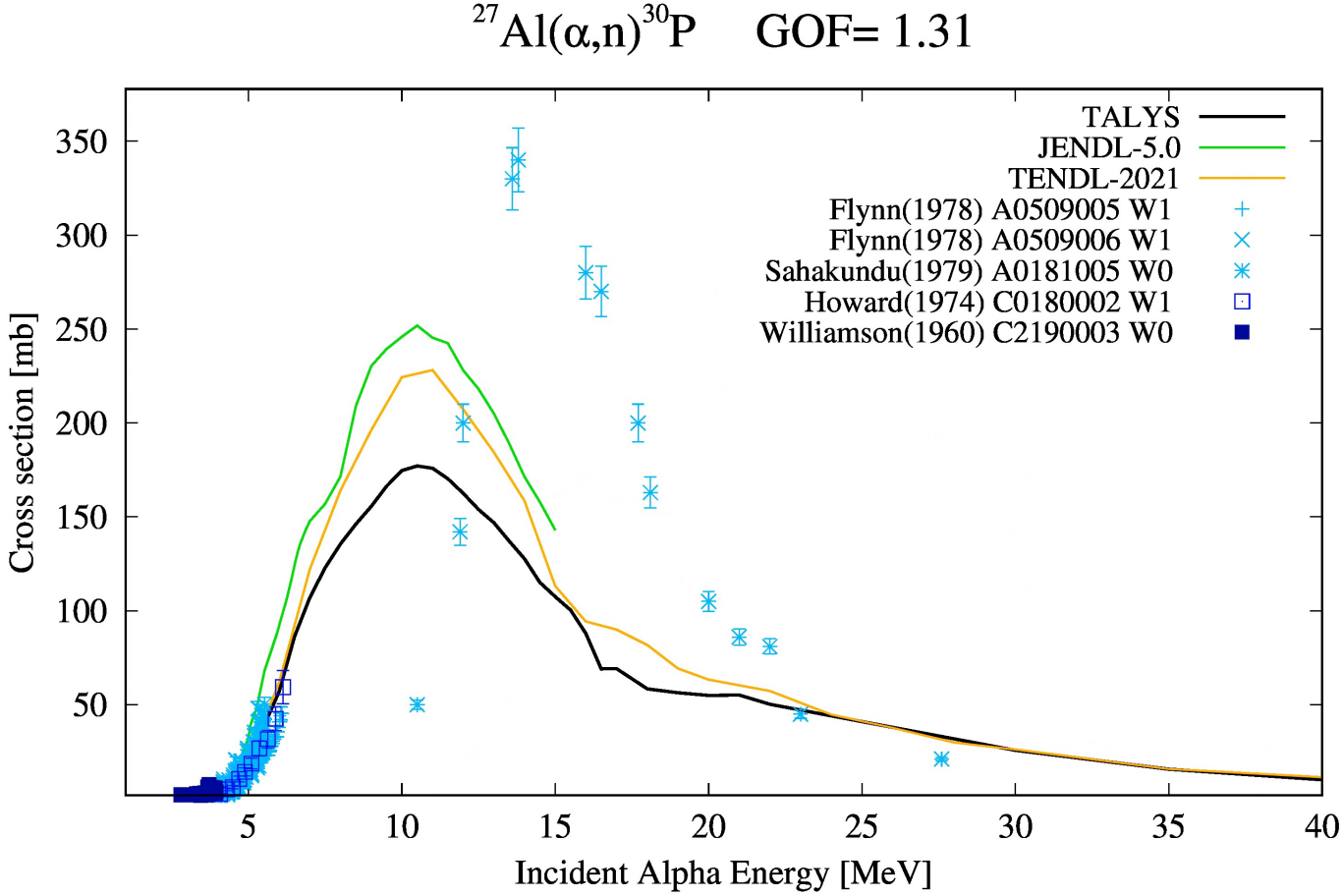


Scouting the nuclear lanscapes





- (α,n), (n,α) and (p,n) films



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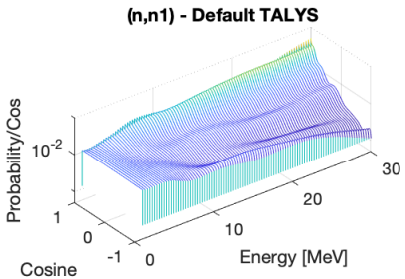
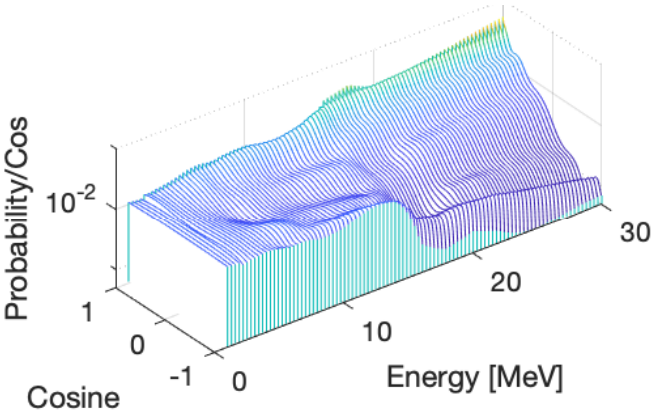
TALYS default, optimized MF1 parameters

- to xs, 0.0253 eV
- to MACS, 30 Kev
- to Maxw., SPA
- to xs, < 1 MeV
- to angles
- …




```
                Adjusted TALYS input parameters                    2631 1451
#                                                                  2631 1451
# General                                                          2631 1451
#                                                                  2631 1451
ldmodel 2                                                          2631 1451
#                                                                  2631 1451
# (n,tot), (n,el), (n,inl)                                         2631 1451
#                                                                  2631 1451
awdadjust n 1. awdadjust-n.table                                   2631 1451
#                                                                  2631 1451
# (n,p), (n,2n), (n,np)                                            2631 1451
#                                                                  2631 1451
rvadjust p 0.99                                                    2631 1451
avadjust p 0.99                                                    2631 1451
gnadjust 26 57 0.90                                                2631 1451
gpadjust 26 57 0.90                                                2631 1451
aadjust 25 56 1.12                                                 2631 1451
pshiftadjust 26 56 -0.2                                            2631 1451
pshiftadjust 25 56 0.1                                             2631 1451
#                                                                  2631 1451
# (n,a)                                                            2631 1451
#                                                                  2631 1451
cknock a 1.1                                                       2631 1451
cstrip a 1.1                                                       2631 1451
#                                                                  2631 1451
# (n,g)                                                            2631 1451
ldmodelCN 1                                                        2631 1451
#                                                                  2631 1451
# Other: Isomers, (n,d), (n,t), (n,h) etc.                         2631 1451
#                                                                  2631 1451
***************************** T A L Y S ***************************2631 1451
```



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TENDL-2023 ASTRO

- 8892 isotopes for astrophysics applications: cross sections, reaction rates and MACS
- Different reaction "model sets" were used: "a model set" represents a combination of up to 9 TALYS models, not all are compatible:

1. Gamma strength function (values 8 or 9): either Gogny D1M HFB+QRPA, or SMLO
2. Level density (values 1, 2 or 5): Constant temperature + Fermi gas model, or Back-shifted Fermi gas model, or Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables
3. JLM microscopic optical model potential or KD optical model (values y or n)
4. Gamma strength function for M1 (values 3 or 8): Hartree-Fock BCS tables or Gogny D1M HFB+QRPA
5. Collective enhancement (values y or n): yes or no
6. Width fluctuation (values 0, 1 or 2): Moldauer or Hofmann-Richert-Tepel-Weidenmueller model
7. Mass model (values 0, 1, 2 or 3): Duflo-Zuker formula, Moeller table, Goriely HFB-Skyrme table, or HFB-Gogny D1M table (except for known masses, where the experimental value is used)
8. Alpha optical model (values 5 or 6): Demetriou/Goriely, or Avrigeanu
9. Fission model (values 1 or 5): "experimental" fission barriers, or WKB approximation for fission path model.

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TENDL-2023 ASTRO https://tendl.web.psi.ch/tendl_2023/astro/astro.html

- Started August 10th, 2022 and still goin on…
- 200 cores, up to 480 model combinations (x2 for fissiles) x isotopes x 4 metrics

TENDL-astro 2023

Cross sections, reaction rates and MACS for astrophysics

Recommended quantities

Quantities with uncertainties

	10 models	480 models (A< 210)	960 models (A≥210)
1. cross sections:	(n,g) (n,p) (n,a)	(n,g) (n,p) (n,a)	(n,g) (n,p) (n,a)
2. cross sections:	(p,g) (p,n) (p,a)	(p,g) (p,n) (p,a)	(p,g) (p,n) (p,a)
3. cross sections:	(a,g) (a,n) (a,p)	(a,g) (a,n) (a,p)	(a,g) (a,n) (a,p)
4. reaction rates:	(n,g) (n,p) (n,a)	(n,g) (n,p) (n,a)	(n,g) (n,p) (n,a)
5. reaction rates:	(p,g) (p,n) (p,a)	(p,g) (p,n) (p,a)	(p,g) (p,n) (p,a)
6. reaction rates:	(a,g) (a,n) (a,p)	(a,g) (a,n) (a,p)	(a,g) (a,n) (a,p)
7. Normalization function:	G(T)	G(T)	G(T)
8. Maxwellian Averaged (n,g) :	MACS	MACS	MACS

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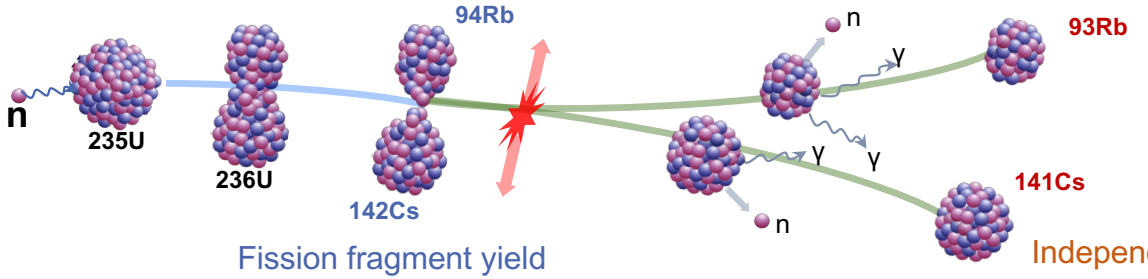
TALYS: prompt fission observable and fission yields



- TALYS treats a fission fragment as an excited nucleus and applies the Hauser-Feshbach statistical decay to the fission fragment de-excitation (prompt decay) and loops over all fission fragments.

Fission fragment generator

Monte Carlo
- GEF (ffmodel1)
- FREYA (ffmodel5?)

Micro/Macroscopic Theory
- SPY model (ffmodel3)
- 4D Langevin by TokyoTech (ffmodel4?)

Phenomenological
- Wahl systematics
- Katakura systematics
- Experimental data fitting (ffmodel2)

Charge distribution
- Z_P model

Energy sorting
- Energy sharing hypothesis

TALYS

Model parameters → Reaction simulations → Multiple emissions → Output

Nuclear structure (RIPL-3)
- Masses, abundance
- Discrete levels
- Level densities
- Neutron resonances
- Fission barrier parameter
- Photon strength function

Optical model (ECIS)
- Phenomenology local/global optical model

Compound reaction
- Hauser-Feshbach
- γ-ray cascade
- Exclusive channels
- Recoils

Fission observables
- PFNS, PFGS (LAB frame conversion, Maxwellian ratio)
- nu n, g
- Yield

Fission fragments
-Mass, charge, yield, excitation energy

Compound reaction
- Width fluctuations
- Gilbert-Cameron + Ignatyuk
- γ-ray emission

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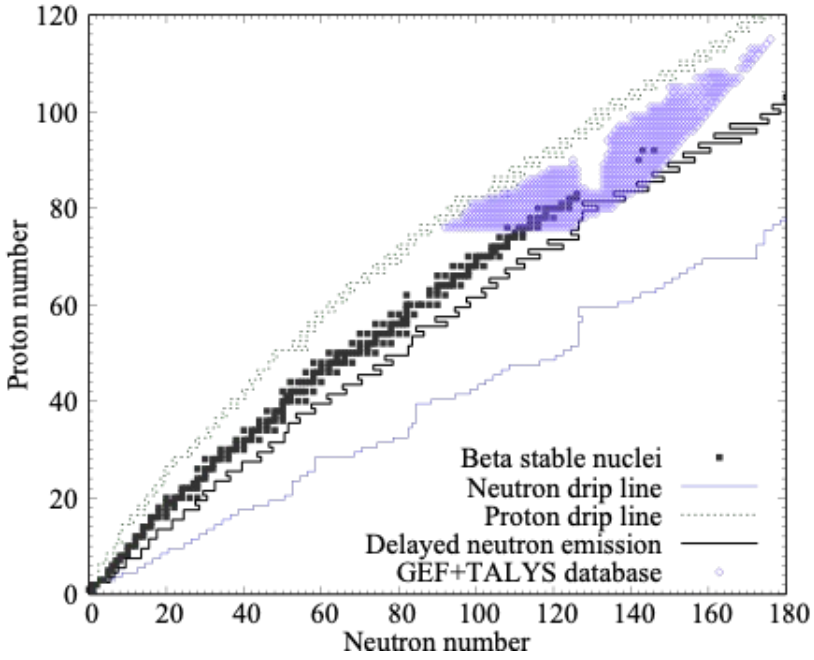
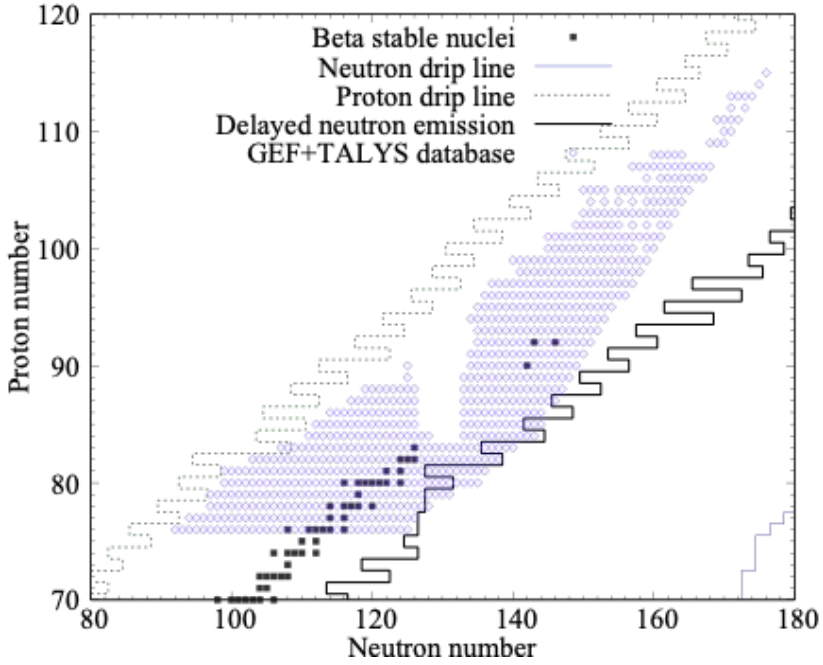
Prompt fission observable and fission yields

- GEF version 2021/1.1 was used -- details are explained in Ref.[1] and [2].
- GEF fission fragment database in TALYS is available for 737 nuclei with 20 excitation energies for each.
- TALYS interpolates yield and excitation energy if the input energy is in between available energies.





[1] F. Nordstrom, Benchmark of the fission channels in TALYS. UPTEC ES 21016, Uppsala University. (2021)
[2] K. Fujio et al., IAEA-NDS-0239 (2022) and EPJ A

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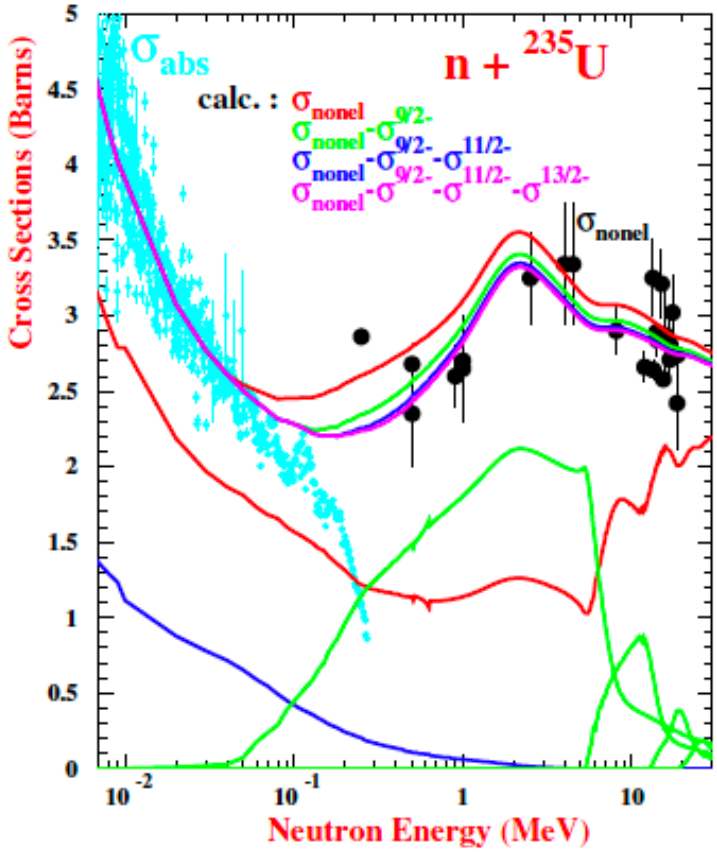
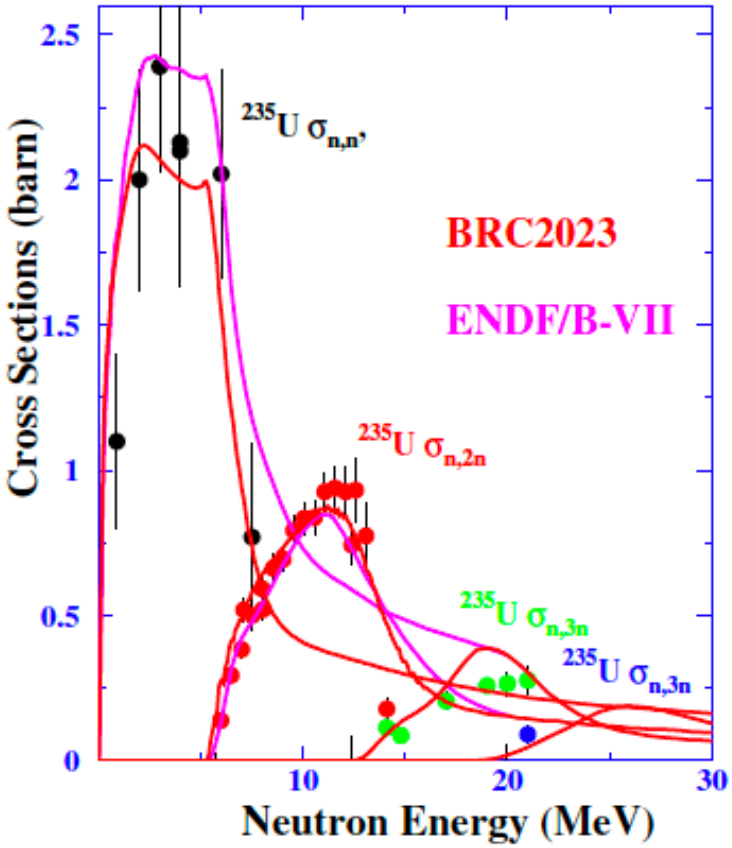
Model updates

- New inelastic scattering model using the Engelbrecht-Weidenmuller Transformation (E-W T)

JEFDOC 2252

Next n-^{238}U !!





TENDL-2023 innovation

- Usage of an enhanced, complete, resonance parameter database
- Major update of the experimental differential and integral databases
- Covariances information on all seven incident particles
- Re-written, modernized codes
- Autotalys default parameters script enhancement, verification

```
$autotalys -element Na -mass 24 -proj n -E30 -nocovar >&  n-Na024.log
```

- 200 cores times 2 months, Swiss power @ PAUL SCHERRER INSTITUT PSI
- …

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Application Portal

Processed through NJOY2016,CALENDF and PREPRO2023 in application libraries for:

- FISPACT-II & CINDER (Bateman solver)
- MCNP6®, TRIPOLI4®, SERPENT,

OpenMC, CASMO and FLUKA (Boltzmann transport solver)

- SPECTRA-PKA (material sciences toolkit)
- …

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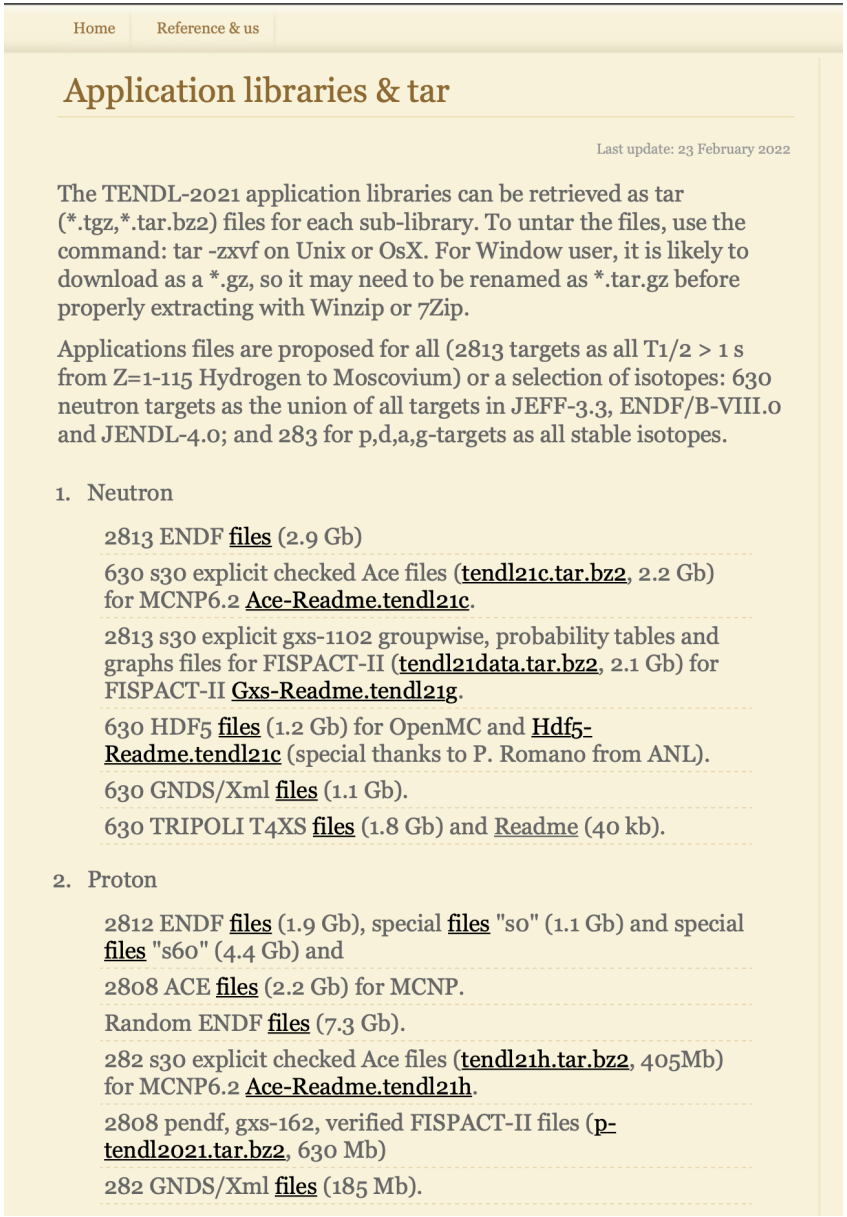

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Application libraries & tar

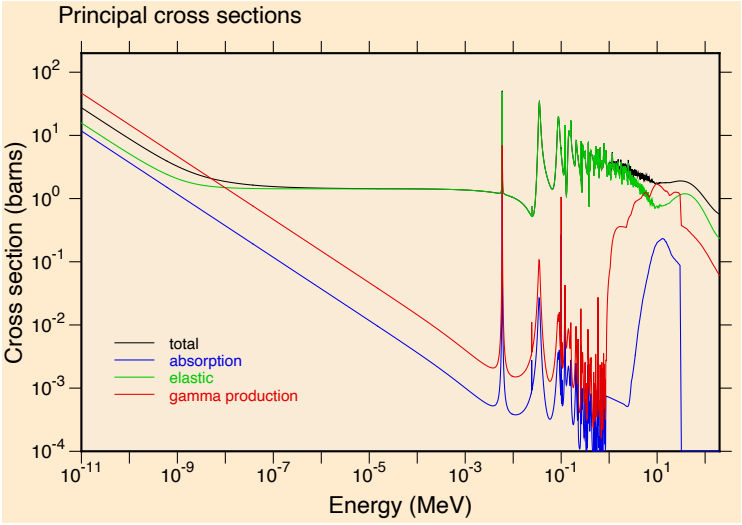
Last update: 23 February 2022

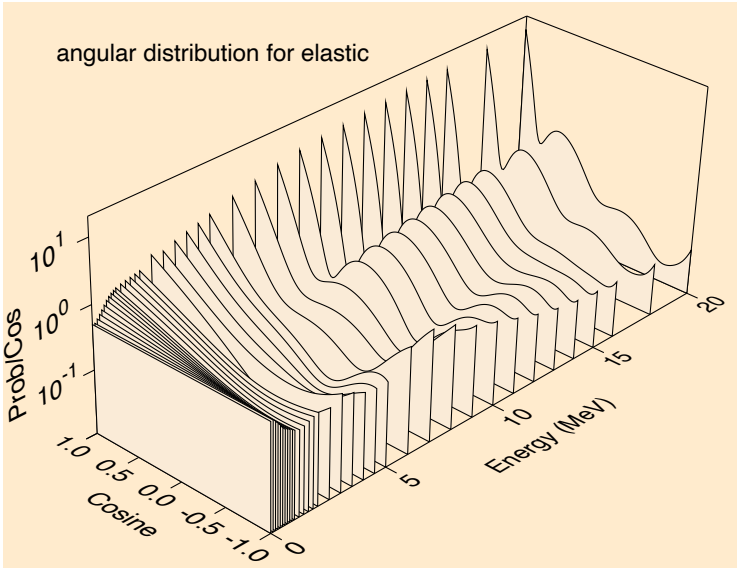
The TENDL-2021 application libraries can be retrieved as tar (*.tgz,*.tar.bz2) files for each sub-library. To untar the files, use the command: tar -zxvf on Unix or OsX. For Window user, it is likely to download as a *.gz, so it may need to be renamed as *.tar.gz before properly extracting with Winzip or 7Zip.

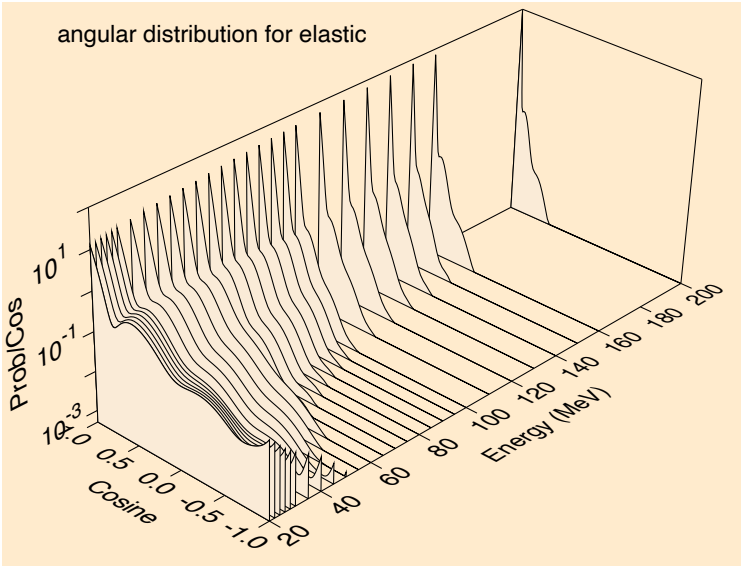
Applications files are proposed for all (2813 targets as all T1/2 > 1 s from Z=1-115 Hydrogen to Moscovium) or a selection of isotopes: 630 neutron targets as the union of all targets in JEFF-3.3, ENDF/B-VIII.0 and JENDL-4.0; and 283 for p,d,a,g-targets as all stable isotopes.

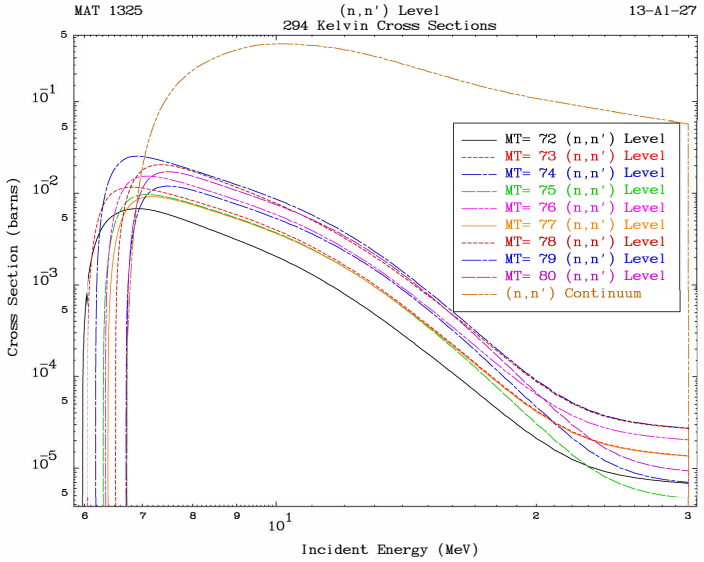
1. Neutron
   - 2813 ENDF files (2.9 Gb)
   - 630 s30 explicit checked Ace files (tendl21c.tar.bz2, 2.2 Gb) for MCNP6.2 Ace-Readme.tendl21c.
   - 2813 s30 explicit gxs-1102 groupwise, probability tables and graphs files for FISPACT-II (tendl21data.tar.bz2, 2.1 Gb) for FISPACT-II Gxs-Readme.tendl21g.
   - 630 HDF5 files (1.2 Gb) for OpenMC and Hdf5-Readme.tendl21c (special thanks to P. Romano from ANL).
   - 630 GNDS/Xml files (1.1 Gb).
   - 630 TRIPOLI T4XS files (1.8 Gb) and Readme (40 kb).
2. Proton
   - 2812 ENDF files (1.9 Gb), special files "s0" (1.1 Gb) and special files "s60" (4.4 Gb) and
   - 2808 ACE files (2.2 Gb) for MCNP.
   - Random ENDF files (7.3 Gb).
   - 282 s30 explicit checked Ace files (tendl21h.tar.bz2, 405Mb) for MCNP6.2 Ace-Readme.tendl21h.
   - 2808 pendf, gxs-162, verified FISPACT-II files (p-tendl2021.tar.bz2, 630 Mb)
   - 282 GNDS/Xml files (185 Mb).

Applications forms









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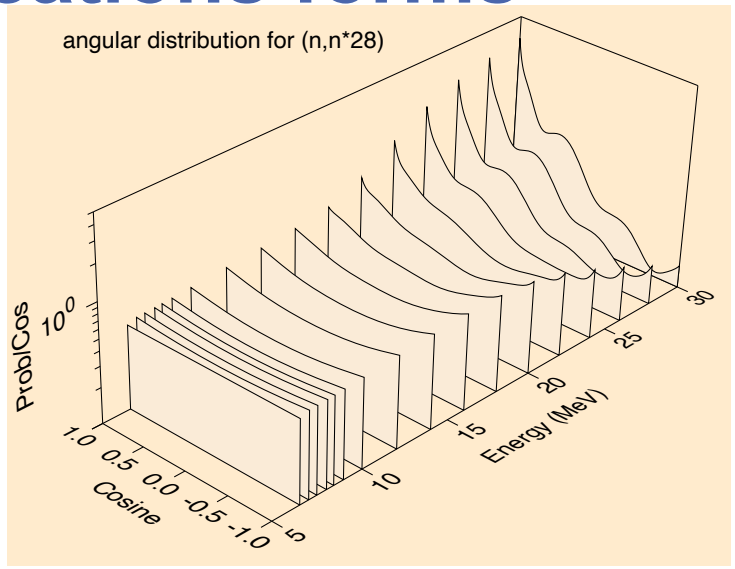
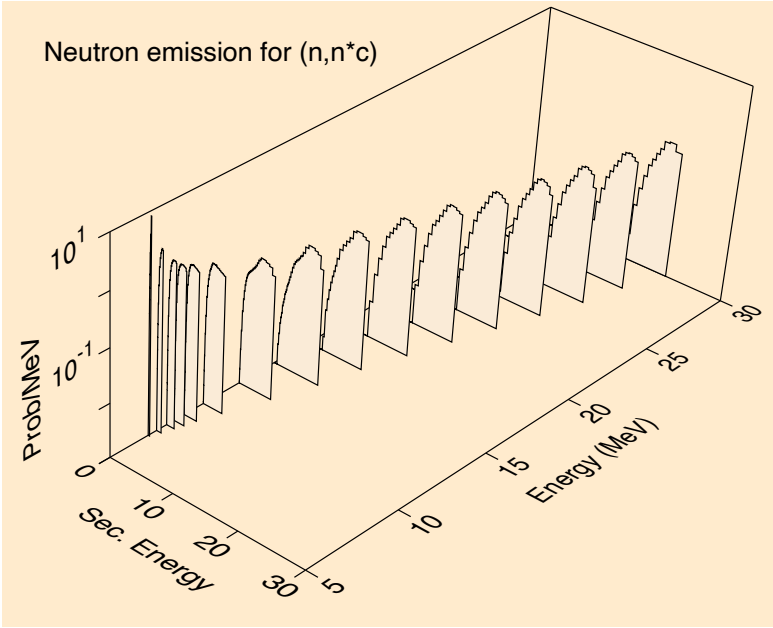
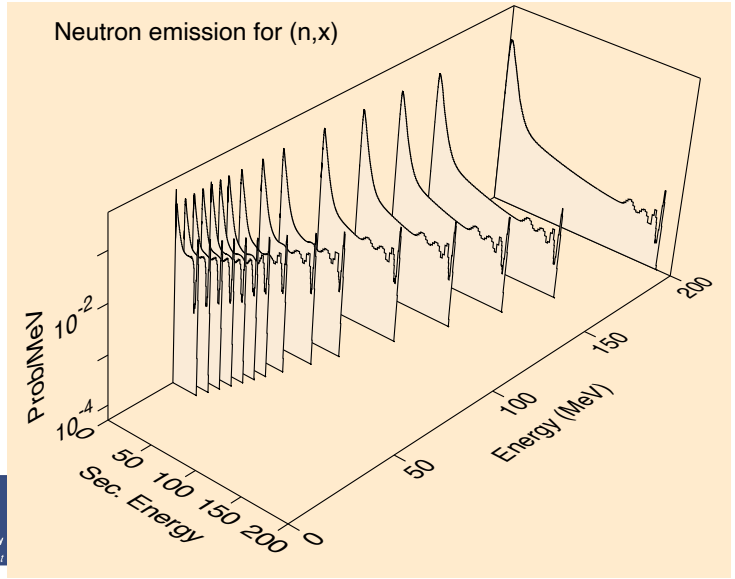
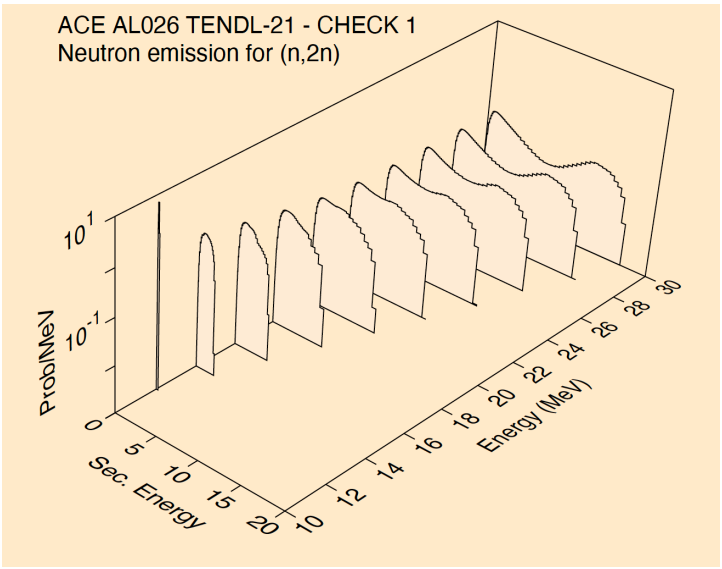
Applications forms









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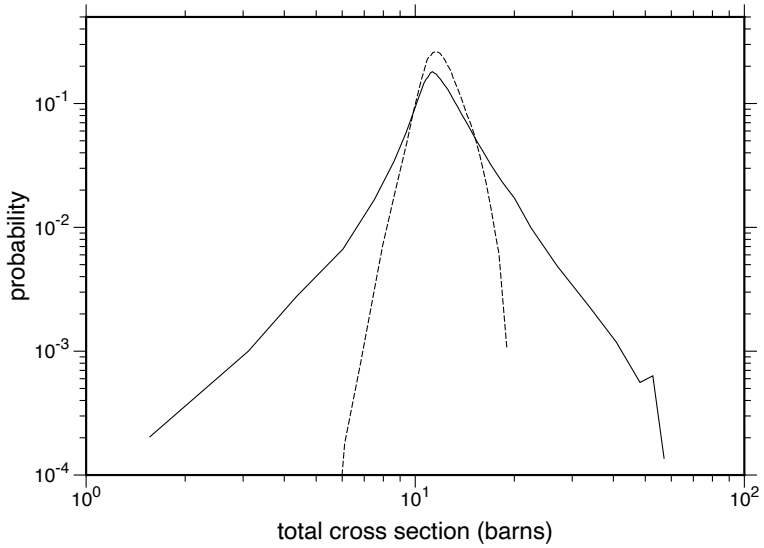
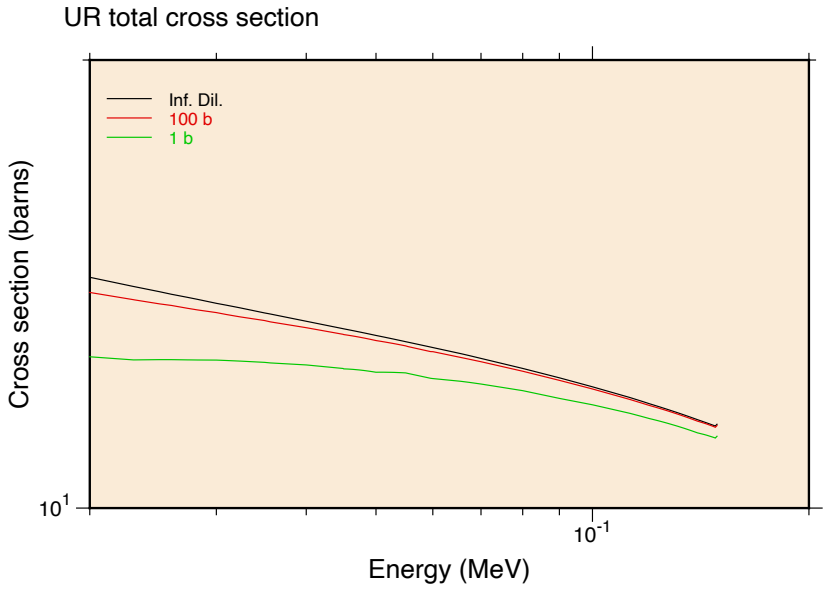
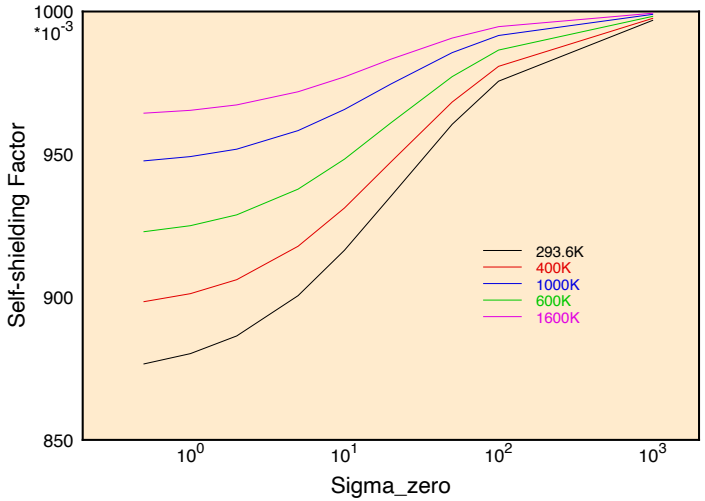
Applications forms

- U238
- PDFs @ 20 keV, dashed 140 keV

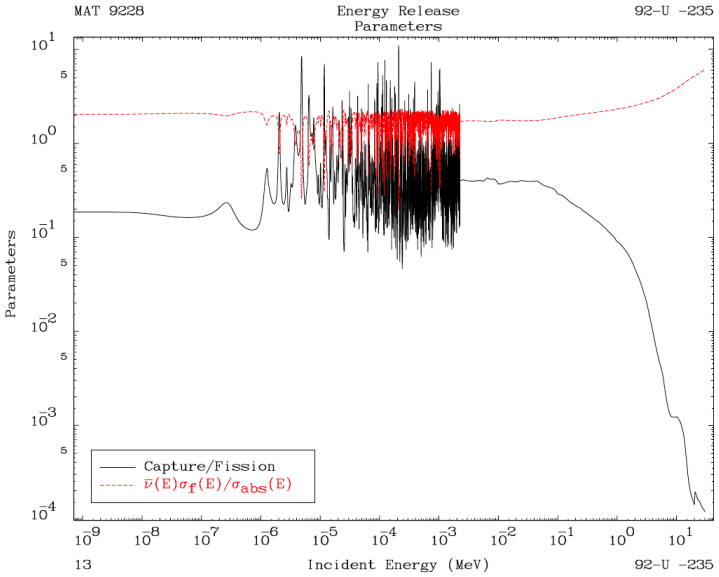


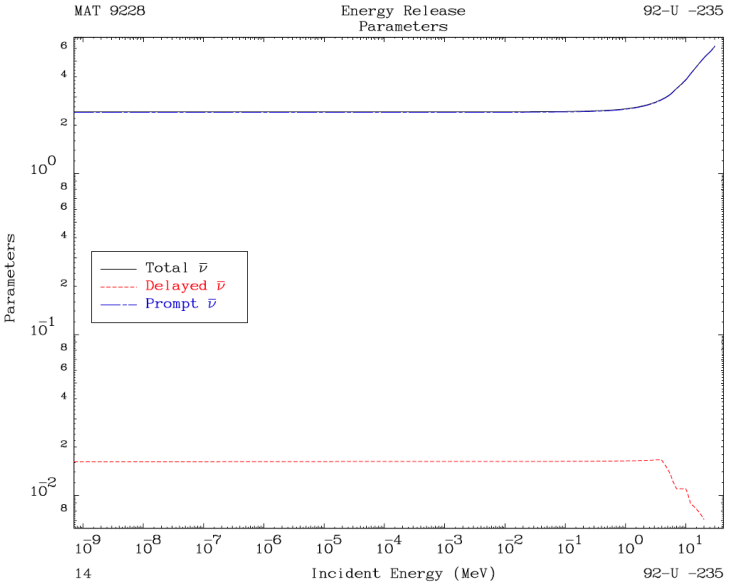


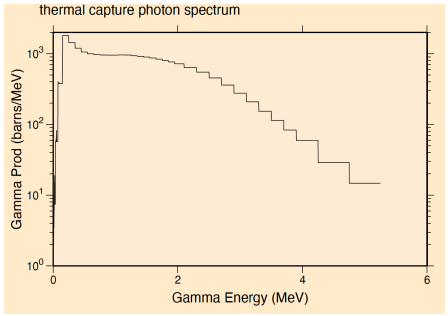


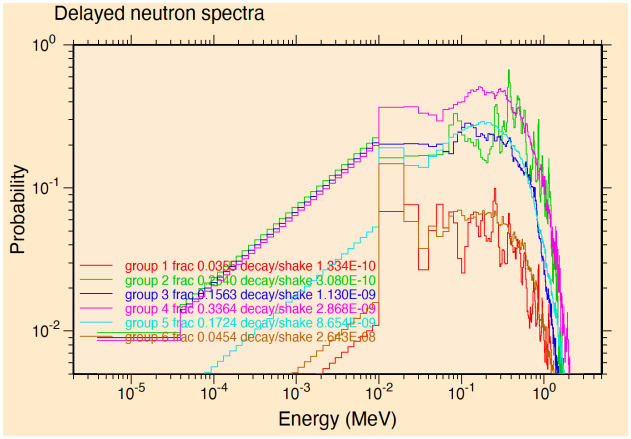
Reactor physics lexical : background (dilution)

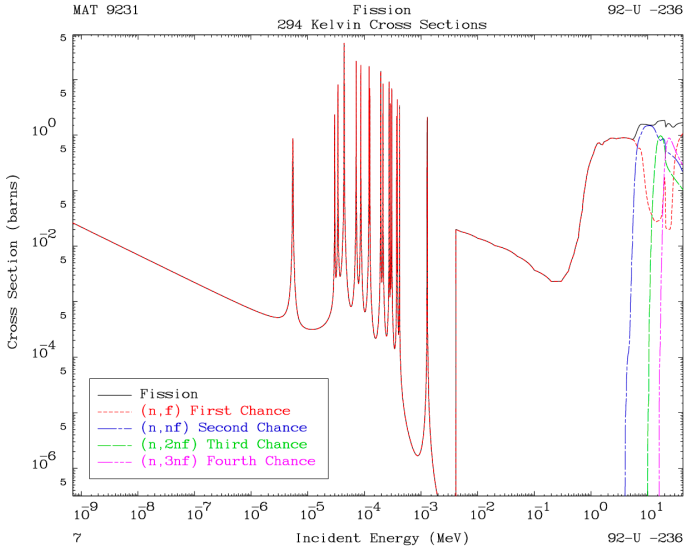
Applications forms











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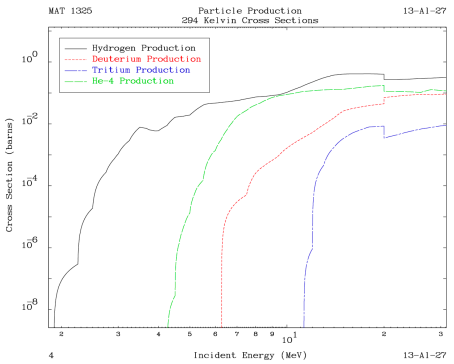
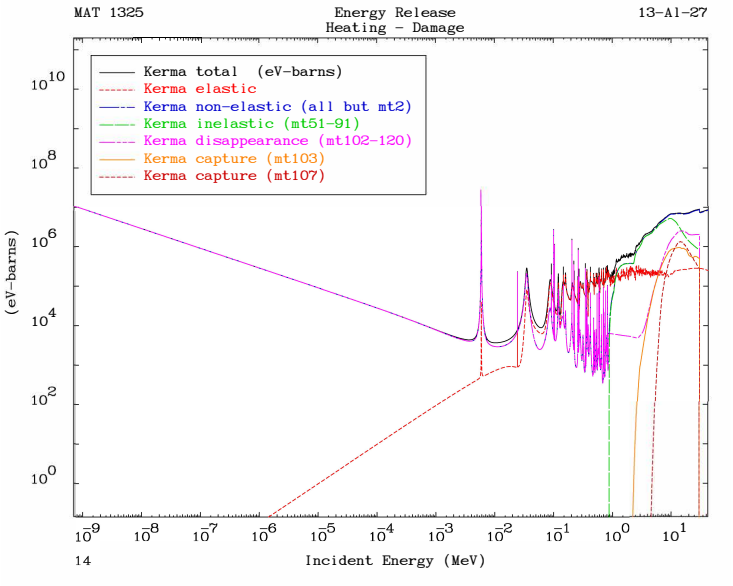
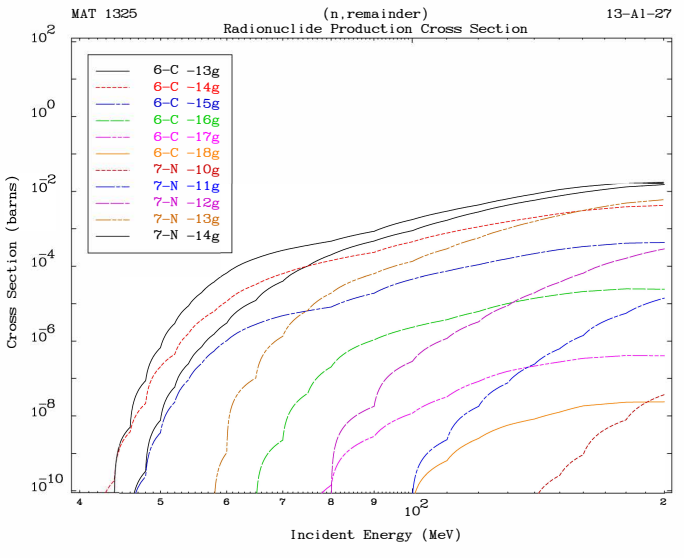
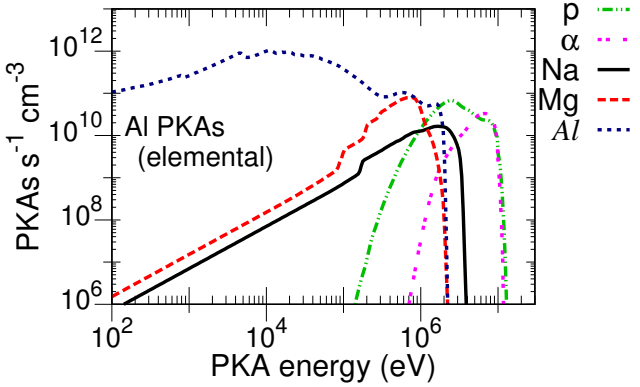
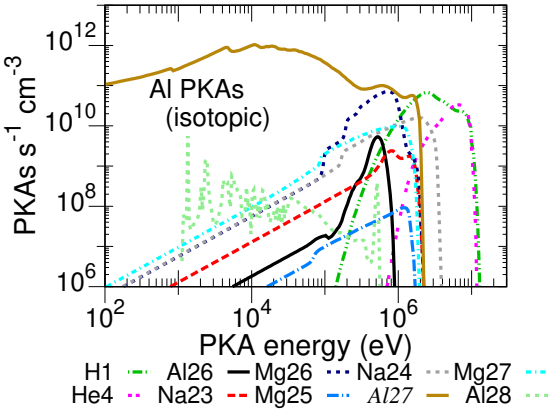
Applications forms



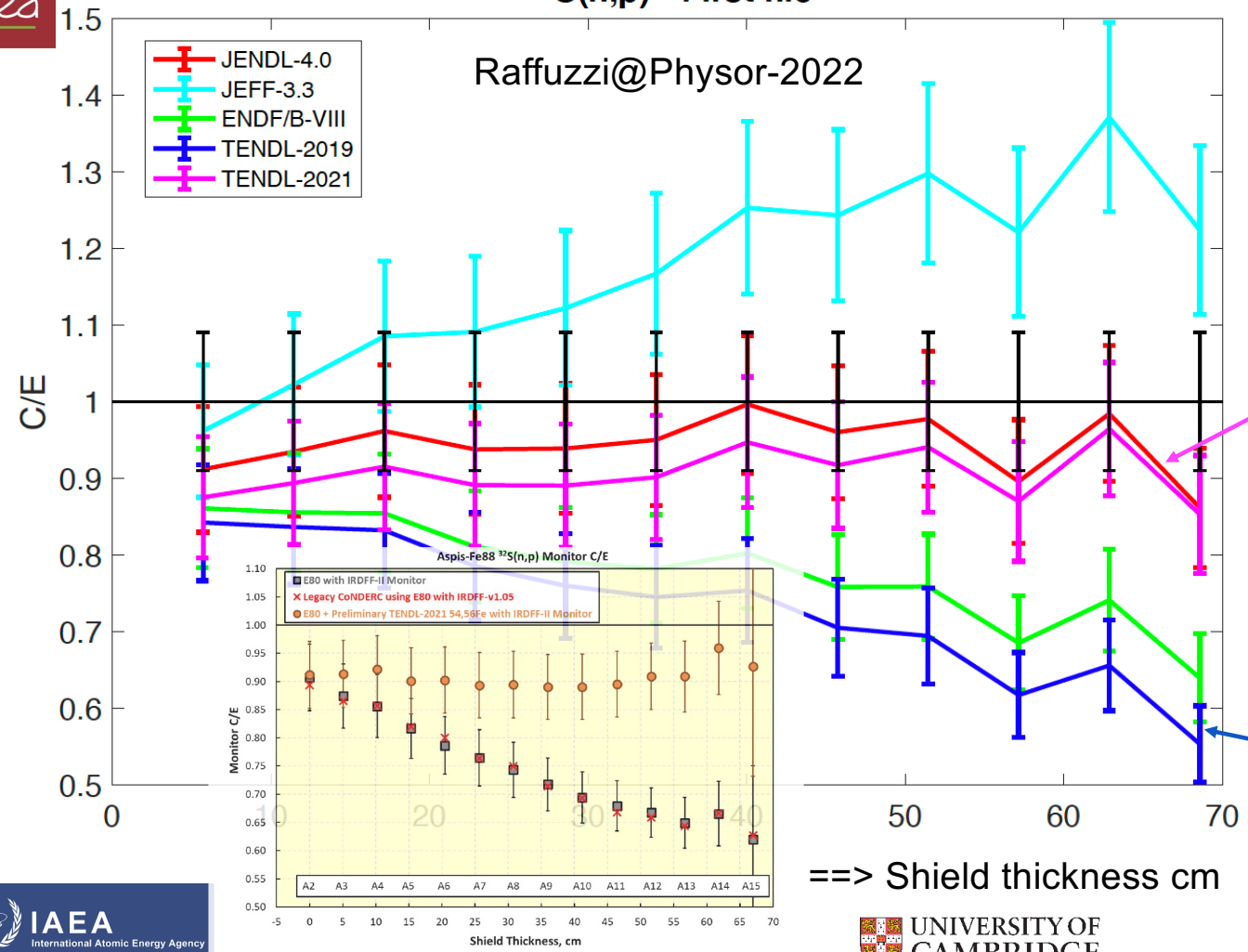


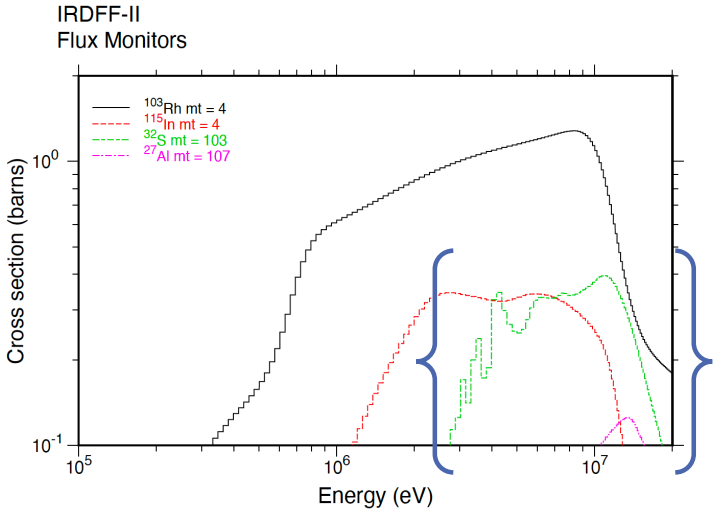




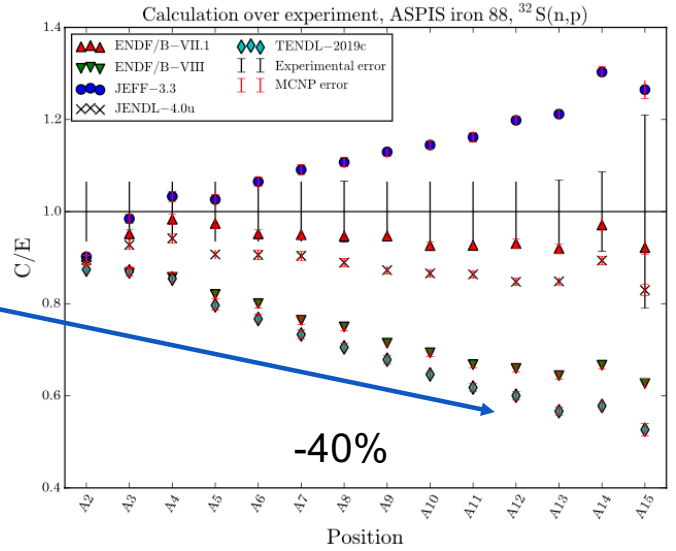


V&V TRIPOLI4® & MCNP6® Shielding ASPIS





TENDL-21 as performant as JENDL-4 and without background



==> Shield thickness cm

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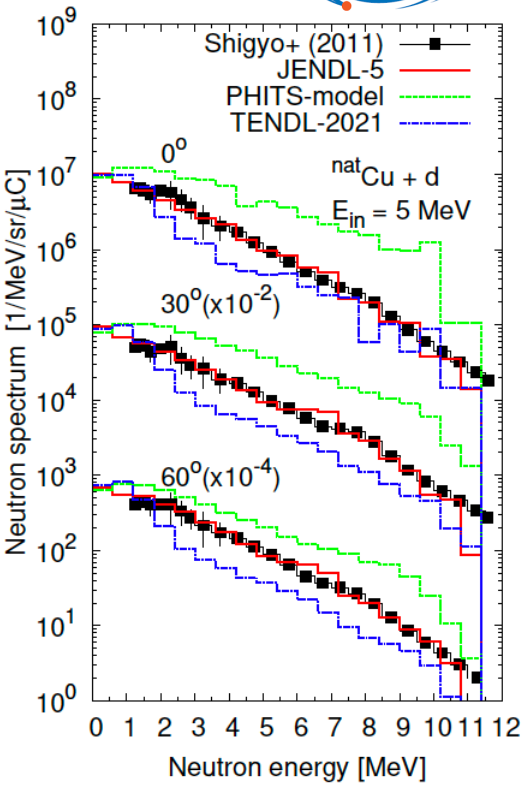
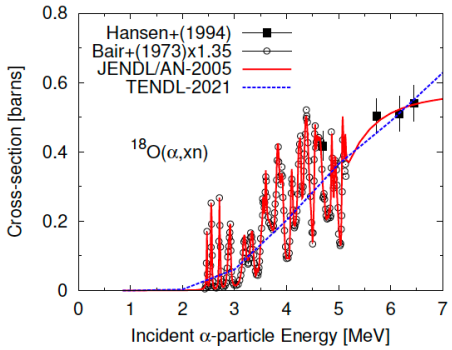
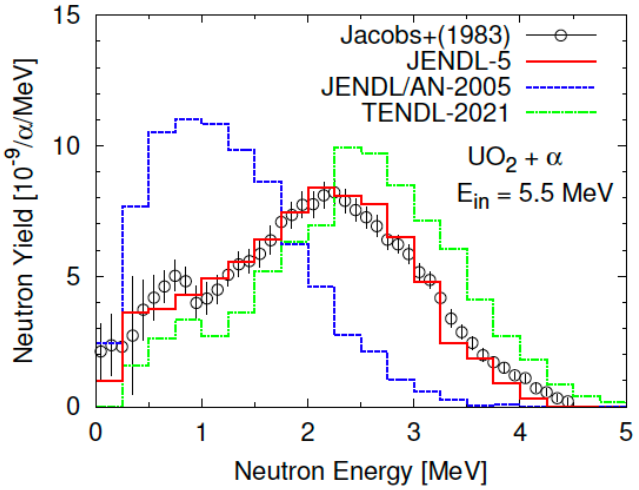
CP's V&V deuteron, alpha, gamma induced libraries

- 5 MeV deuteron on thick Copper

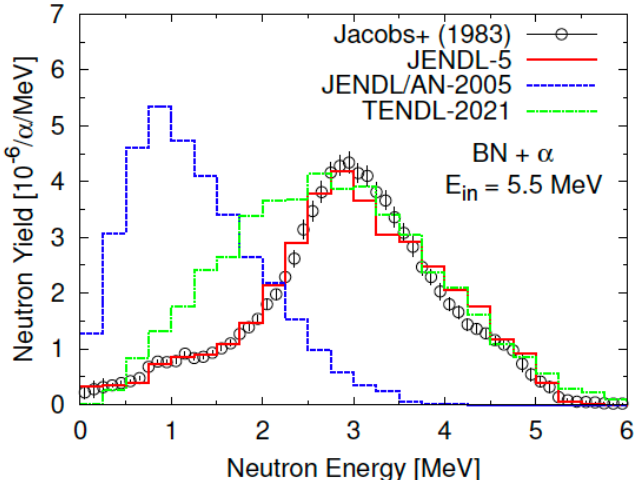






- 5.5 MeV alpha on UO_2 and Boron nitride

Do application need s30 for CP's ?
s15 may seem more resoneable !



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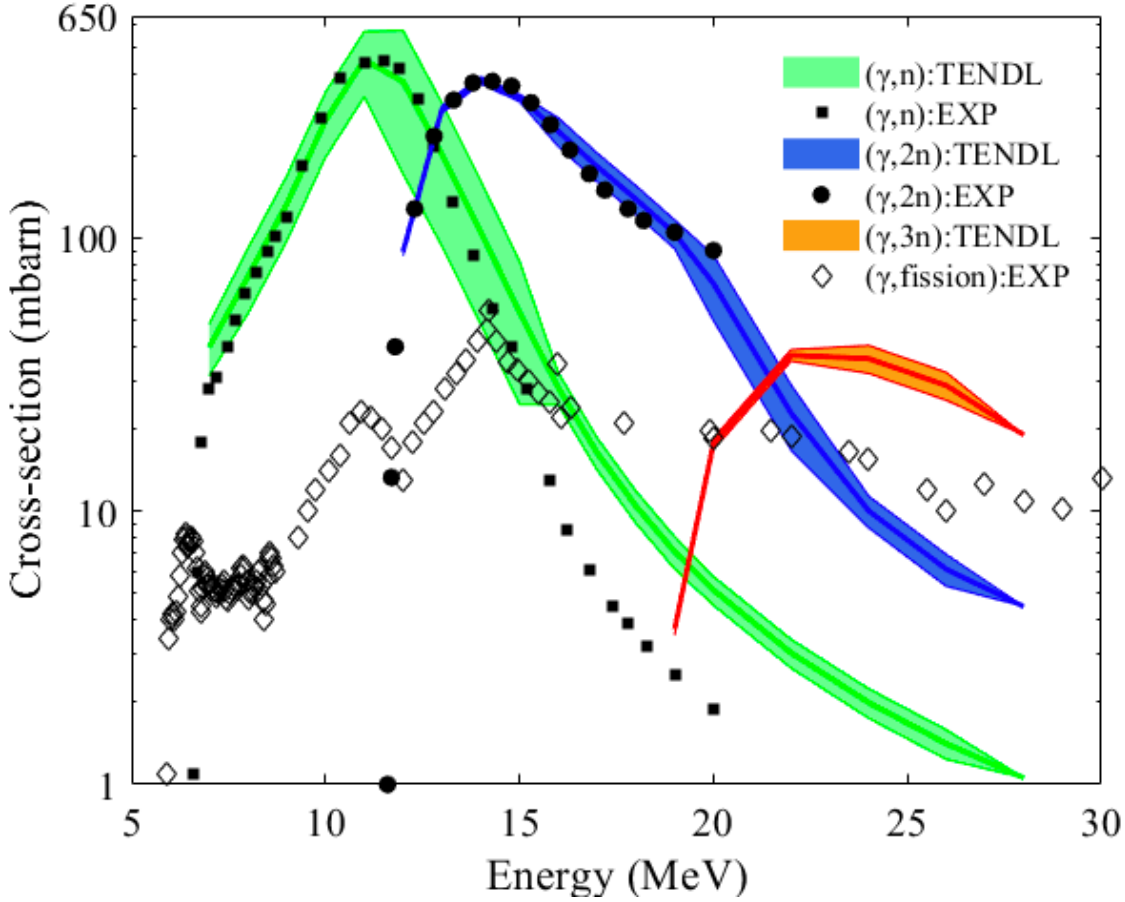
CP's V&V deuteron, alpha, gamma induced libraries

- Gamma on ^{232}Th



- Caveat: KAIST did not tought to look for fission in MF=10 !!

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European Physical Journal A publication

TALYS: Modeling of nuclear reactions

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Abstract

Purpose: TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. **Methods:** A general overview of the implemented physics and capabilities of TALYS is given. The general nuclear reaction mechanisms described are the optical model, direct reactions, compound nucleus model, pre-equilibrium reactions and fission. The most important nuclear structure models are those for masses, discrete levels, level densities, photon strength functions and fission barriers. **Results:** A wide variety of nuclear reactions simulated with TALYS will be demonstrated, ranging from low-energy neutron cross sections, astrophysics, high-energy charged particle reactions and other reactions. **Conclusion:** TALYS is a nuclear reaction software which aims to give a complete description of nuclear reaction observables, and to be an important link between fundamental nuclear physics and applications.

Keywords: TALYS, nuclear reaction, nuclear structure, cross section, optical model, compound nucleus, pre-equilibrium, level density, photon strength function, fission, astrophysics

MSC Classification: 25.40.-h , 24.10.Ht , 24.60.Dr , 24.10.Pa

Workshop: https://indico.ictp.it/event/10221

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smr3887@ictp.it

Joint ICTP-IAEA Workshop on Simulation of Nuclear Reaction Data with the TALYS Code | (smr 3887)

Starts 16 Oct 2023
Ends 20 Oct 2023
Central European Time

ICTP
Giambiagi Lecture Hall (AGH)
Riva Massimiliano e Carlotta, Grignano
I - 34151 Trieste (Italy)

Organizers

Arjan KONING (IAEA, Austria), Local Organiser: Nadia Binggeli (ICTP)

Co-sponsors

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The call for applications is open. Please click on 'Apply here' to submit your application.

An ICTP-IAEA meeting

The purpose of the workshop is to provide training and information exchange for nuclear physicists, nuclear engineers, and other users of nuclear data for nuclear applications. The Workshop will revolve around TALYS, an open source code for the simulation of nuclear reactions.

TALYS is a nuclear reaction program for the complete and accurate simulation of nuclear reactions up to energies of 200 MeV, through an optimal combination of reliable nuclear models, flexibility and user-friendliness. TALYS can be used for the analysis of basic nuclear reaction experiments or to generate nuclear data for applications. Currently, there are more than 6000 publications in which TALYS is used, for applications such as astrophysics, medical isotope production, fission and fusion energy applications, and many others. The success of TALYS to simulate cross section and other observables depends on a solid implementation of nuclear reaction and structure models, including the optical model, discrete levels, level densities, fission, photon strength functions.

Topics:

- General principles of nuclear reaction and nuclear structure physics
- Measurements of nuclear reaction data, the variety of experimental data and adjusting TALYS nuclear model parameters to obtain good fits to experiment
- Modern theoretical nuclear structure and reaction models, application of TALYS results in nuclear technology and basic nuclear science
- The capability to run TALYS sample cases from low to high energies with hands-on exercises
- Analyses of cross sections, spectra, angular distributions, and fission yields
- Uncertainty quantification

Lecturers:

S. GORIELY, Université Libre de Bruxelles, Belgium
S. HILAIRE, CEA, DAM, DIF, France
A. KONING, IAEA, Austria
S. POMP, University Uppsala, Sweden
D. ROCHMAN, PSI Villigen, Switzerland

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Screenshot

Status

- The essential knowledge is not the TENDL libraries themselves, but rather the numerical databases, parameters and physic models, processes, codes, tools and know-how that go into the automated making of every evaluations of the seven libraries

- TENDL delivers for all nuclear landscapes, application agnostic

- This year (2023) is made off:
  - physic models sampling (480 model combinations x 8892 targets for Astrophysics RR)
  - automated experimental information cross-section shape-shifting parameters set
  - extended, enhanced fission observables
  - Engelbrecht-Weidenmüller transformation implementation
  - updated neutron scattering lengths (TARES)
  - application agnostic detailed (capture, inelastic) prompt gamma ray yields and multiplicity
  - application driven ENDF-6 free physic forms out of TALYS
  - Autotalys, TALYS, TEFAL, TASMAN GitHub distribution
  - …

ENDF, GNDS forms

- Evaluated forms are hybrid specimen assembled from
  - experimental information & R Matrix formalism
  - nuclear model & structure
  - nuclear model & structure & differential tweak
  - nuclear model & structure & differential tweak & integral adjustment
- Evaluated forms are just a commencement, although it is seen as an end by an entire community
- The laws of Physics allow many verification (not validation) processes to take place during the making, assemblage and processing of evaluated file

ENDF, GNDS forms processes

- Processing system convert ENDF, GNDS forms into forms useful for practical applications: fission, fusion, stockpile stewardship, criticality safety, radiation shielding, nuclear medicine procedures, earth, space exploration and more
- 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 to forms useful for applications and well beyond cross-section or criticality studies only

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Thank you for your attention

With the kind participation of: Stephane Goriely, Stephane Hilaire, Pascal Romain, Shin Okumura, Kazuki Fujio and more..