IAEA 60 Years
Atoms for Peace and Development

TALYS and TENDL: status and future

Arjan Koning

Nuclear Data Section
International Atomic Energy Agency, Vienna

Workshop on TALYS/TENDL developments, Prague, Czech Republic, November 13-15, 2017

Contents

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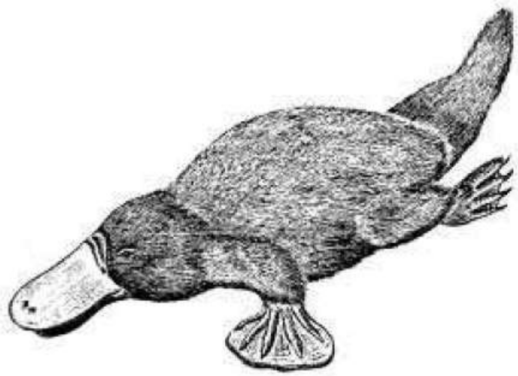
- Status
  - TALYS-1.8/1.9
  - TENDL-2015/2017
- Future
  - TALYS-2.0 and beyond
  - TENDL-2018 and beyond
- Conclusions

TALYS-1.8

New Edition December 26, 2015

A nuclear reaction program

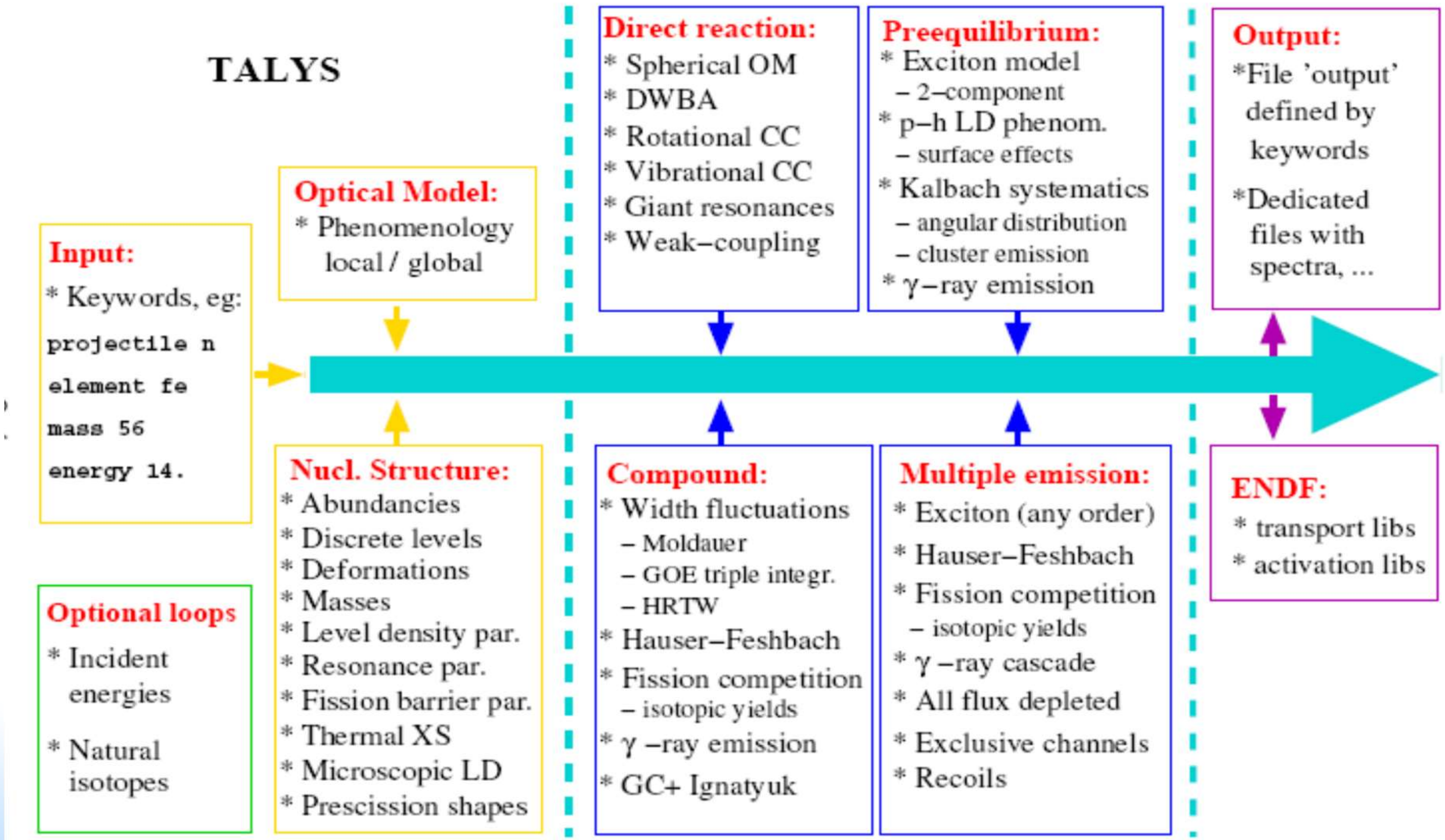


PLATYPUS

User Manual

Arjan Koning
Stephane Hilaire
Stephane Goriely

TALYS code scheme



GENERAL FEATURES
What TALYS yields

Cross sections :

- total, reaction, elastic (shape & compound), non-elastic, inelastic (discrete levels & total)
- total particle production
- all exclusive reactions (n,nd2a)
- all exclusive isomer production
- all exclusive discrete and continuum g-ray production

Spectra :

- elastic and inelastic angular distribution or energy spectra
- all exclusive double-differential spectra
- total particle production spectra
- compound and pre-equilibrium spectra per reaction stage.

Fission observables :

- cross section (total, per chance)
- fission fragment mass and isotopic yields

Miscellaneous :

- recoil cross sections and ddx
- particle multiplicities
- s and p wave functions and potential scattering radius r'
- nuclear structure only (levels, Q, ld tables, …)
- specific pre-equilibrium output (ph lds, decay widths …)
- astrophysical reaction rates

GENERAL FEATURES
TALYS versions online

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http://www.talys.eu

TALYS 1.0 (ND 2007)

TALYS 1.2 (End of 2009)

- new keywords (mainly to improve fitting possibilities)
- bugs corrected to solve crashes or unphysical results
- inclusion of microscopic ph level densities
- inclusion of Skyrme-HFB structure information (def., masses, γ strengths)
- inclusion of D1M

TALYS 1.4 (End of 2011)

- new alpha and deuteron OMP
- URR extension

TALYS 1.6 (End of 2013)

- non-equidistant excitation energy binning possible (extension to energies > 200 MeV)
- direct and semi-direct capture added
- new microscopic level densities from D1M
- medical isotope production implemented
- coupling to GEF for fission yields done

TALYS 1.8 (End of 2015)

- Resolved resonance range added
- More extensive GEF and fission possibilities (PFNS) added

GENERAL FEATURES
Technical details

- Fortran 77 , gradually evolving into full Fortran95

- ≈ 110000 lines (+ 20000 lines of ECIS)

- Modern programming
  - modular (312 subroutines)
  - Explicit variable names and many comments (30% of total number of lines)
  - Transparent programming (few exceptions)

- Flexible use and extensive validation
  - Flexibility : default ⇒ 4 line idiot proof input (element, mass, projectile, energy)
    adjustment ⇒ 400 keywords
  - Random input generation to check stability
  - Drip-line to drip-line calculations help removing bugs

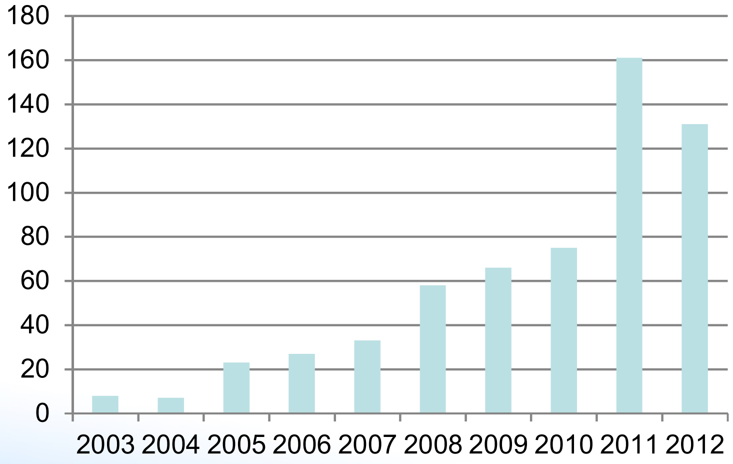
- >500 pages manual

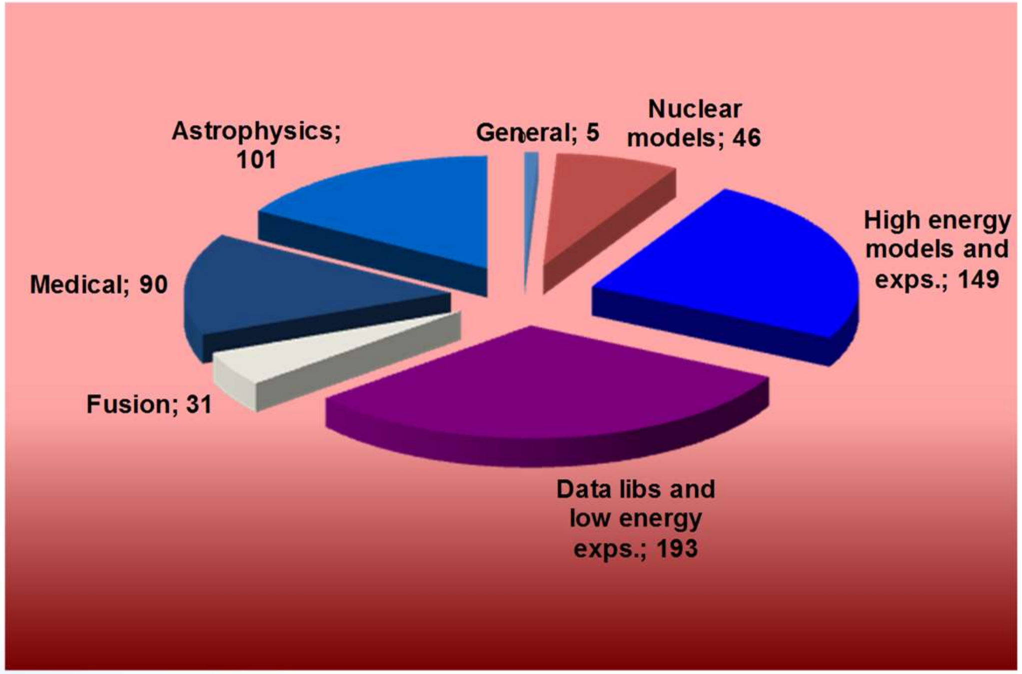
- Compiled and tested with several compilers and OS

TALYS users and publications

- No systematic update done in manual after 2013
- For the new manual: We need a bibtex file with ALL publications that contain TALYS (and/or TENDL)

PUBLICATIONS





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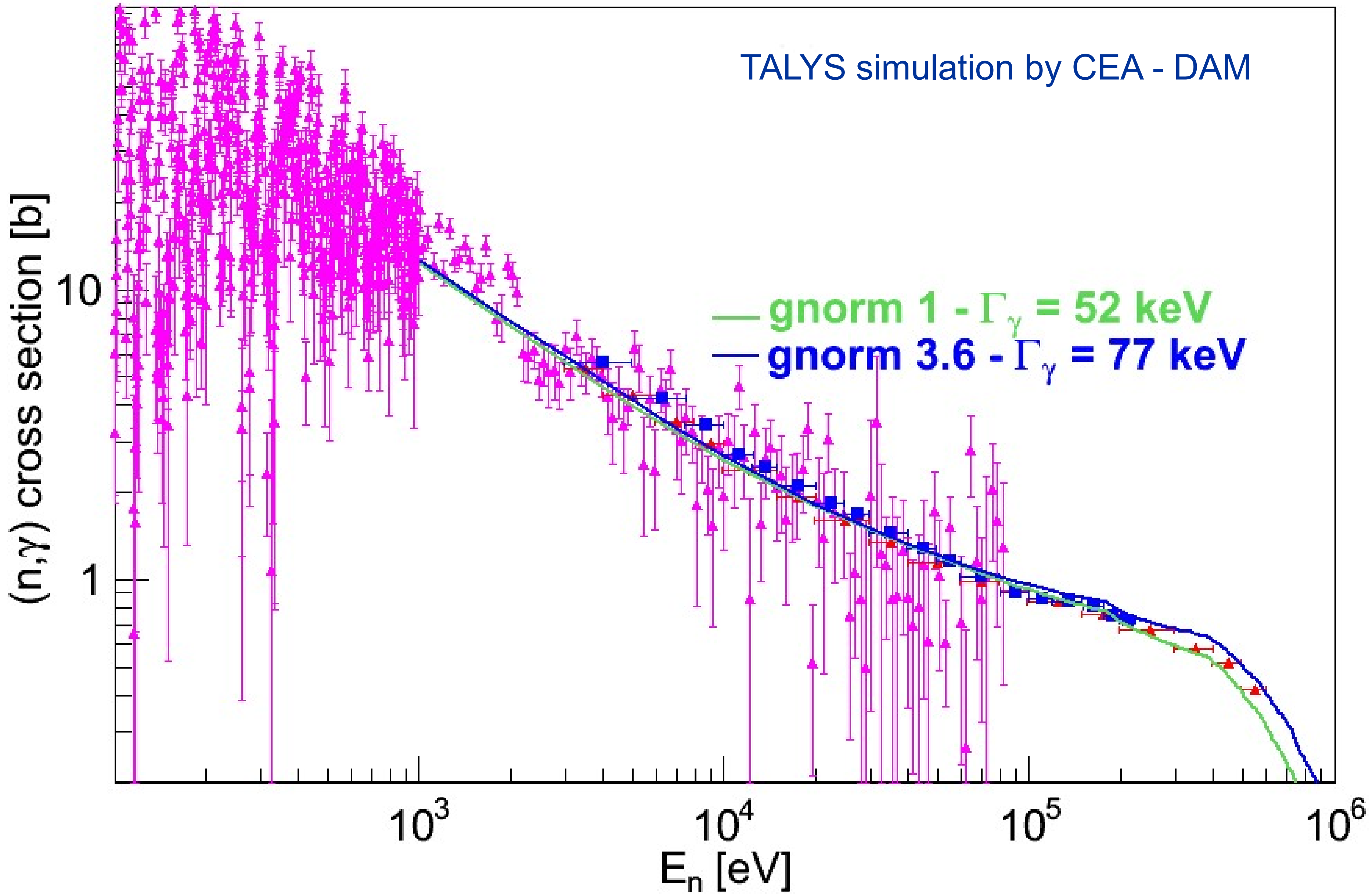
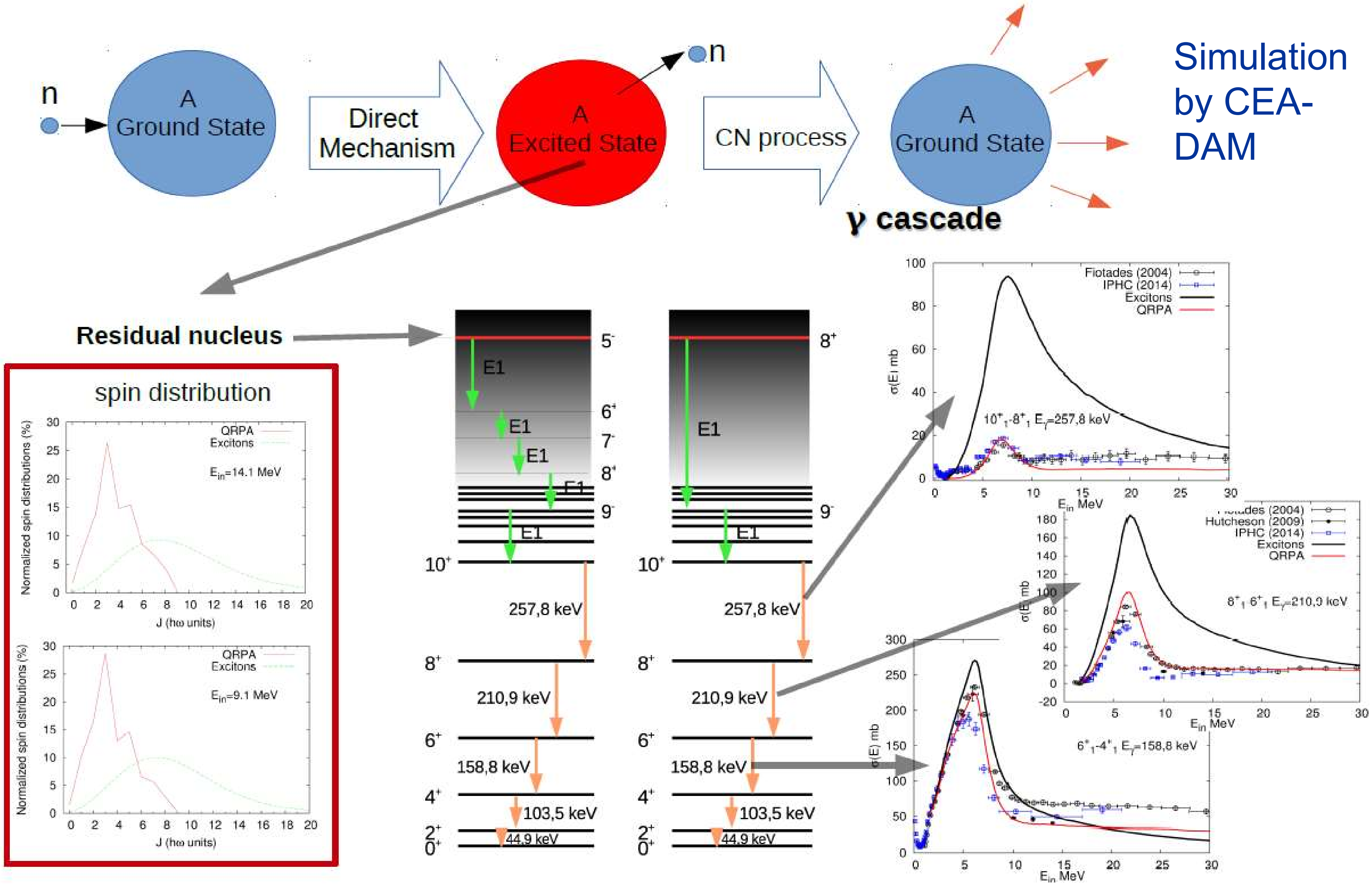
Microscopic / Phenomenologic



Microscopic / Phenomenologic

Simulation by CEA-DAM



TALYS-1.8 reconstructs resonances (Thanks to Red Cullen and PREPRO codes)

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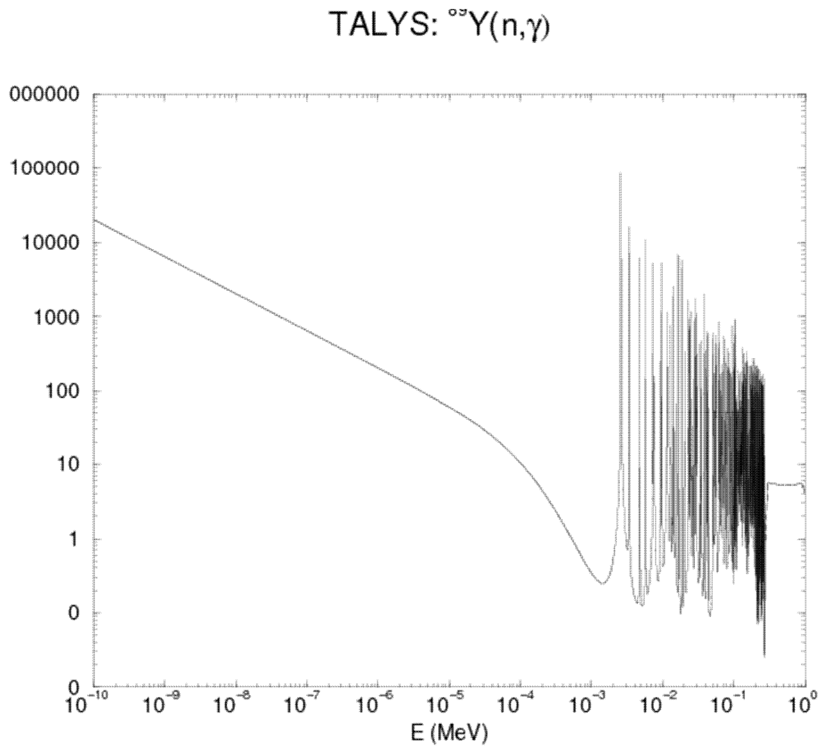

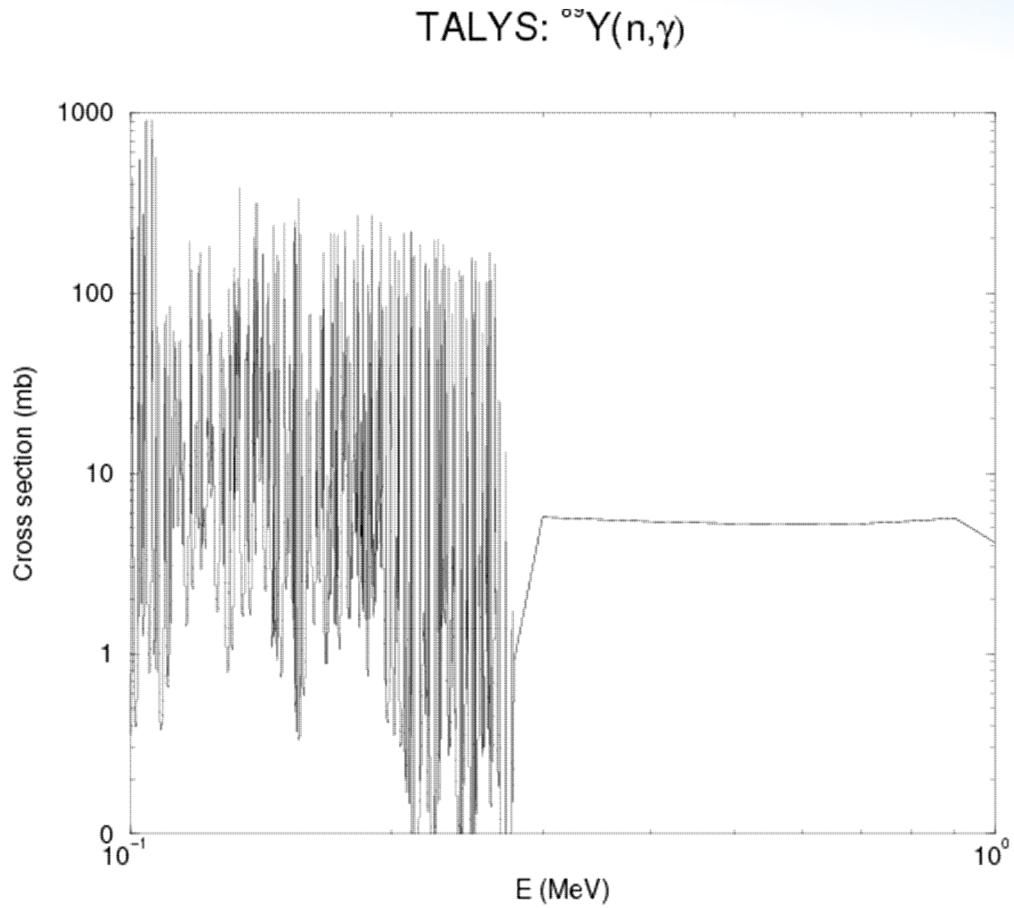

Simulated resonances

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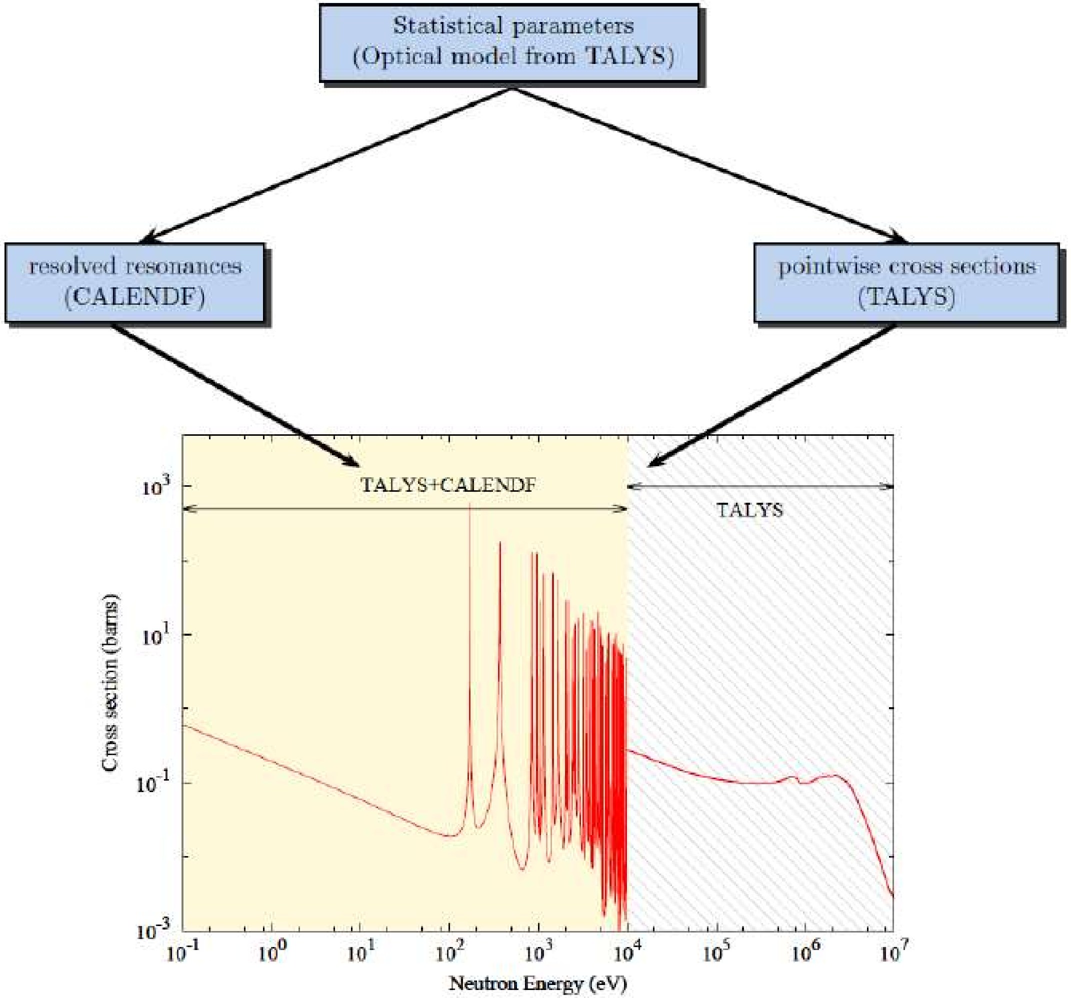
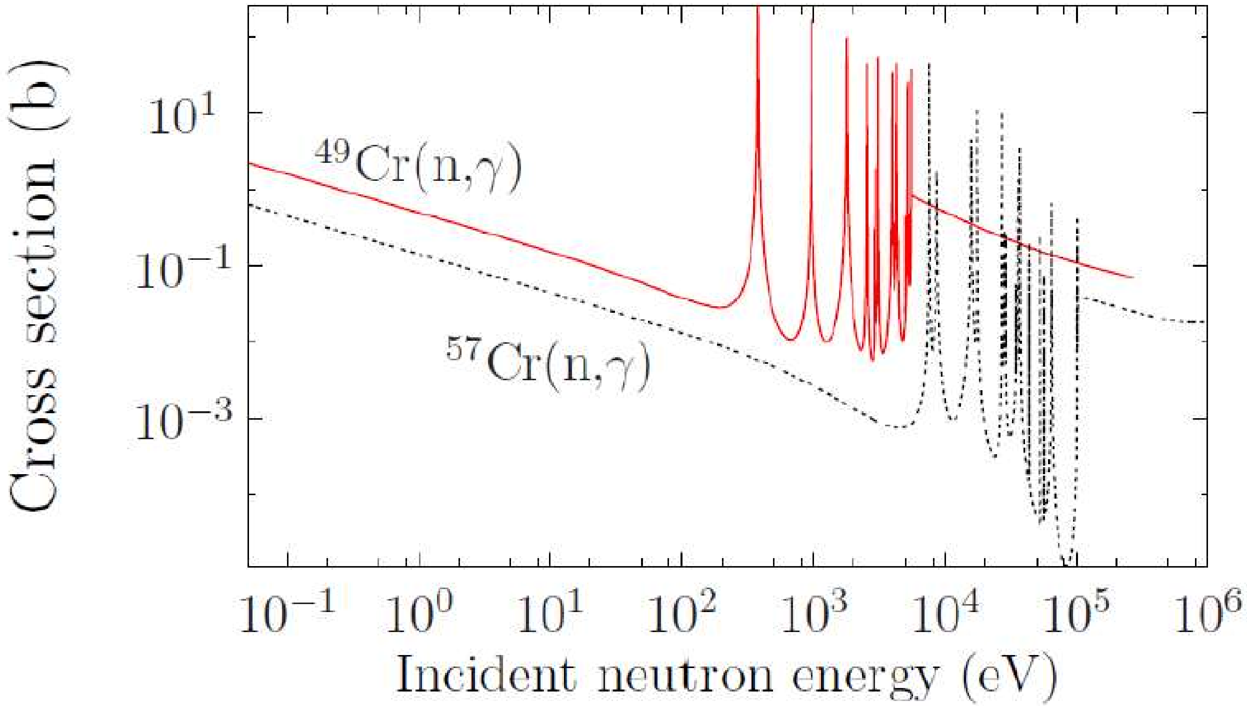
- Alternative approach to the HF calculations: the High Fidelity Resonance calculations (HFR)
- Presented in ANE 50 (2013) 60
  - Combine the 3 previous models (ld, omp and γ-str) to produce statistical resonances
- Uses the following scheme:
  - TALYS (input: ld + omp + γ-str)
  - CALENDF (input: TALYS output)
  - Output: statistical resonances



Simulated resonances

- HFR calculations:
  1. TALYS + specific ld + specific omp + specific γ-str
  2. TALYS output: average D_0, Γ_γ, Γ_n, Γ_f... as a function of E_n
  3. CALENDF + TALYS output in the form of an ENDF-6 file
     - generate random ladders of resonances using the statistical properties
     - Just like in the unresolved resonance range,
     - But this time from 0 to a few 10 or 100 keV.



Maxwellian-Averaged Cross Sections: medium, stable nuclides

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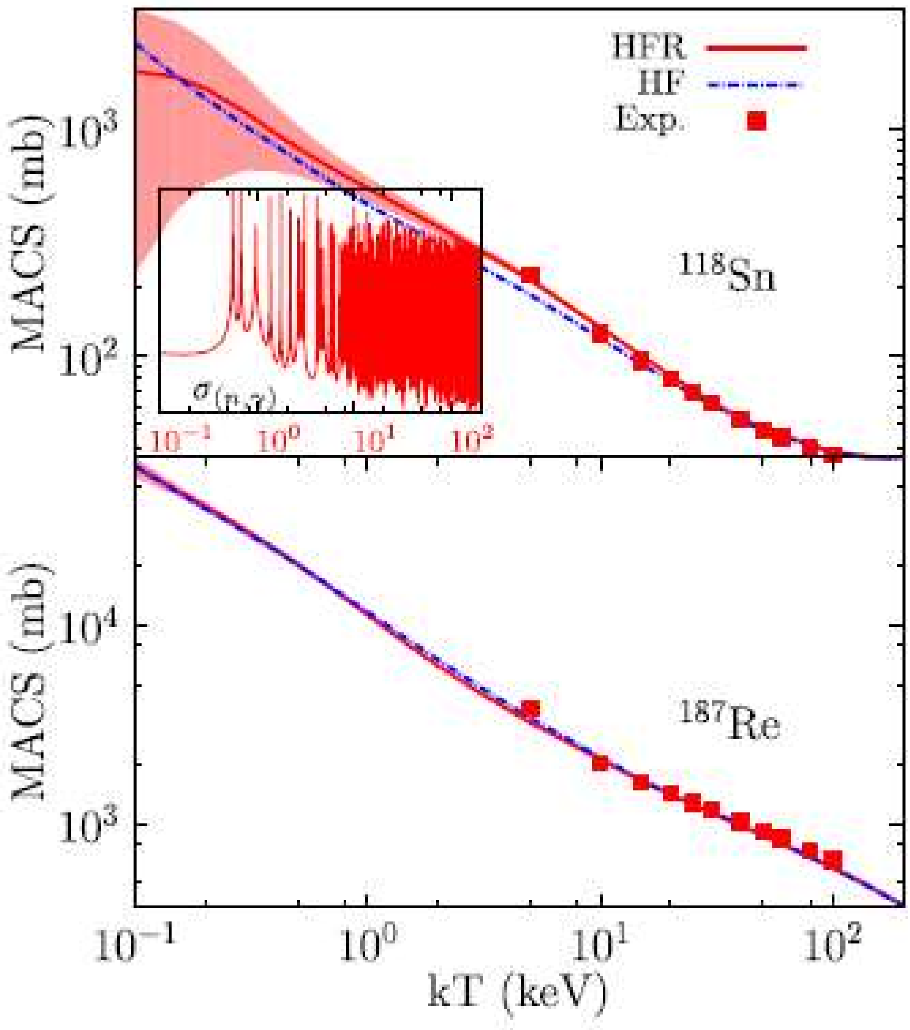
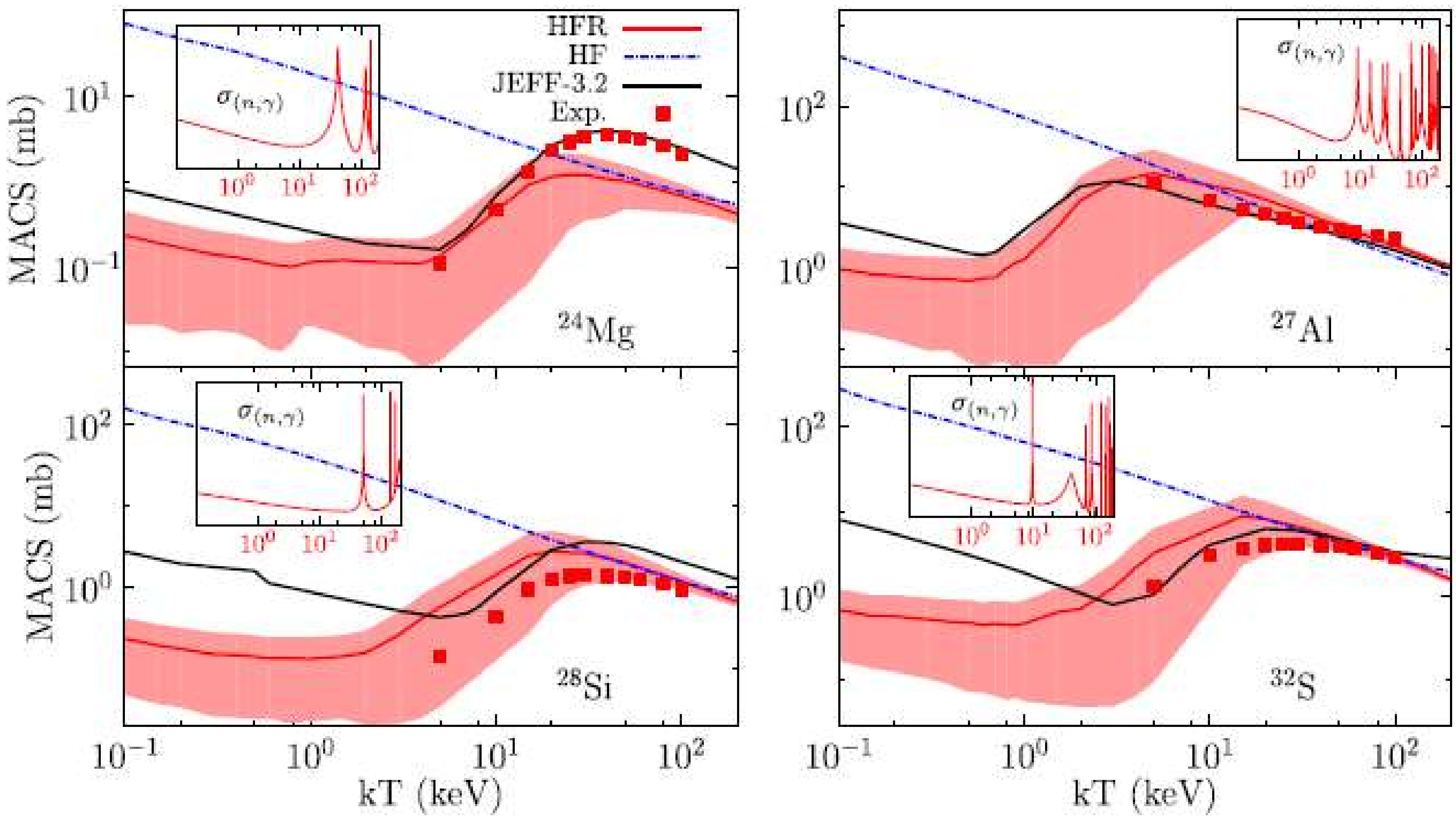
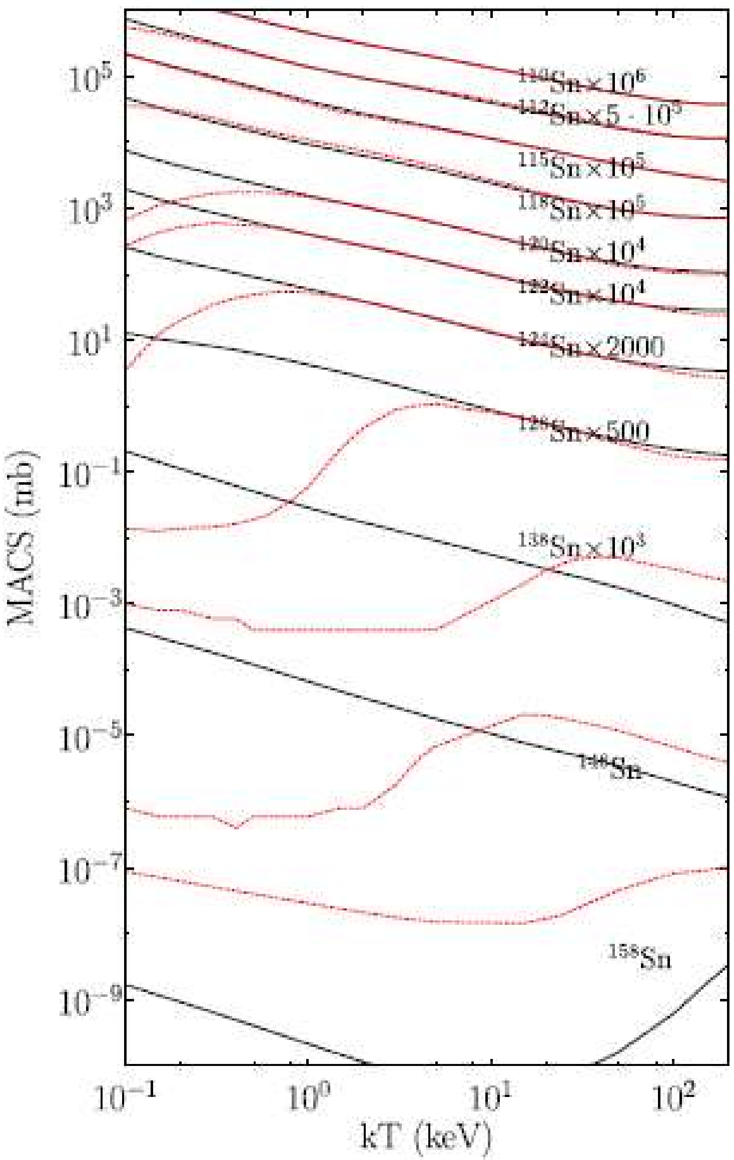


D. Rochman, S. Goriely, A.J. Koning, H. Ferroukhi, "Radiative neutron capture: Hauser Feshbach vs. statistical resonances", Phys. Lett. B764 (2017), 109

Maxwellian-Averaged Cross Sections: light nuclides

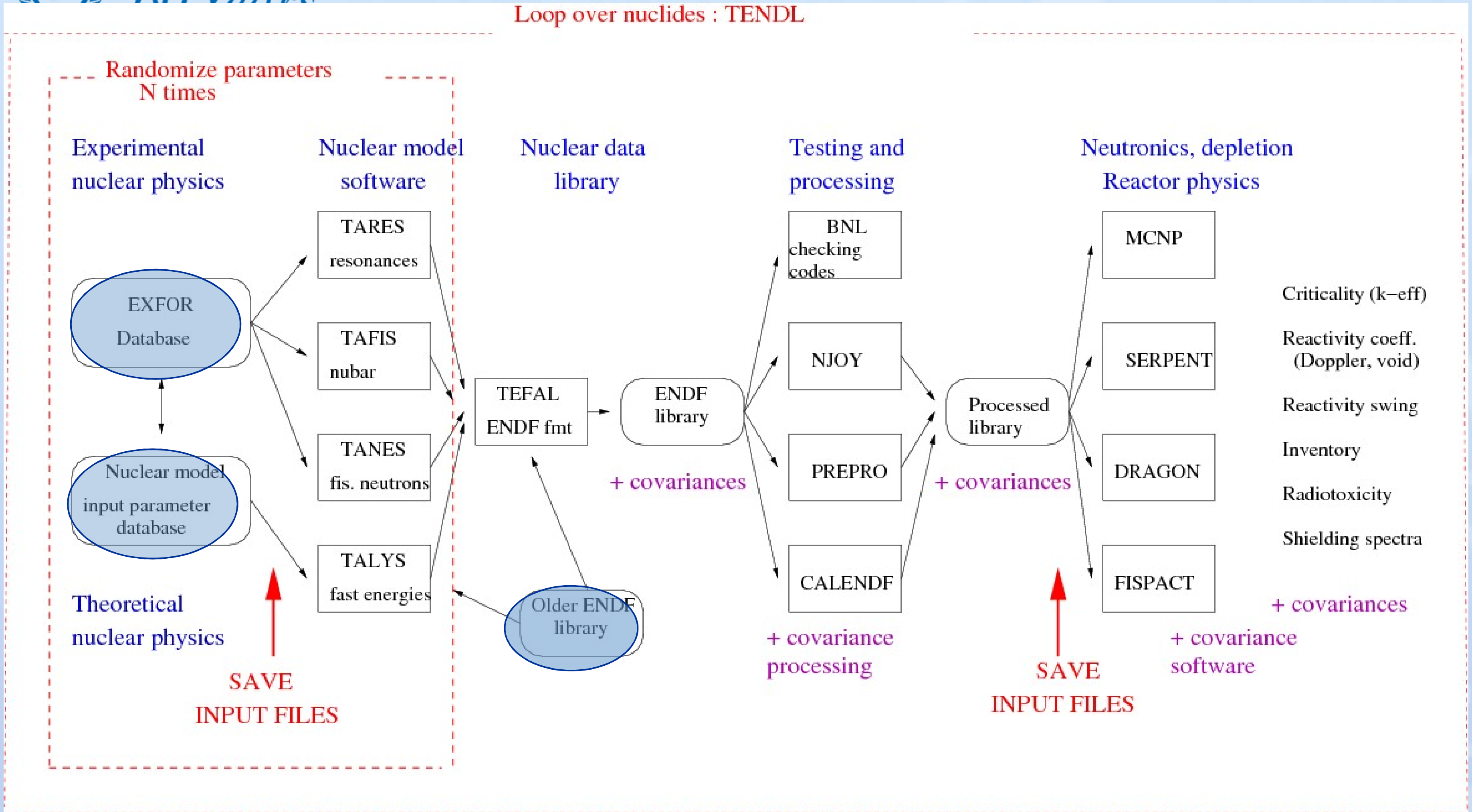


Maxwellian-Averaged Cross Sections:to the dripline



D. Rochman, S. Goriely, A.J. Koning, H. Ferroukhi, “Radiative neutron capture: Hauser Feshbach vs. statistical resonances”, Phys. Lett. B764 (2017), 109

TENDL nuclear data library



A.J. Koning and D. Rochman ,"Modern nuclear data evaluation with the TALYS code system“, Nuclear Data Sheets 113, 2841 (2012).

TENDL philosophy

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- **Fundamental nuclear reaction data should NOT be assembled, or touched, at the level of individual isotopic evaluations of ENDF/B-VII, JEFF, JENDL, CENDL, ROSFOND or CIELO.**
- **Fundamental evaluated nuclear reaction data are:**
  - The EXFOR database with an associated table of weights per experiment
  - An evaluated set of resonance data
  - An input file with parameters for a nuclear model code of a precisely defined version (TALYS-1.8)
  - If necessary: “unphysical actions” like
    - “Fiddling” with data, fit by eye, GLS, other fitting
    - Adoption of MT numbers from existing libraries

    should be stored in scripts
- **TENDL considers ENDF-formatting as trivial and reproducible**
- **Result: fundamental data per isotope are not several Mb in MF1-MF40. The knowledge put into an isotope is represented (and actually is nothing more in practice!) by a few small files. Anything after that: ENDF-6 files, processed files, random files for Total Monte Carlo, etc. etc. is automated.**

TENDL completeness

- All isotopes in the same file structure,
- All to 200 MeV,
- All with covariances (MF-31 to MF40),
- Used in FISPACT-II, CASMO, GEANT,
- 80 isotopes in JEFF-3.2,
- > 300 isotopes in JEFF-3.3beta, 51 isotopes in ENDF/B-VIII

	Neutron	Proton	Deuteron	Triton	Alpha	Helium3	Photon	Fi. Yields	Covariances
TENDL-2015	**2809**	**2804**	**2804**	**2803**	**2804**	**2804**	**2804**	**16**	**2805**
TENDL-2014	**2632**	**2629**	**2629**	**2629**	**2629**	**2629**	**2629**	-	**2632**
TENDL-2013	**2630**	**2625**	**2625**	**2625**	**2624**	**2624**	**2626**	-	**2630**
TENDL-2012	**2435**	**2429**	**2428**	**2348**	**2429**	**2429**	**2430**	-	**2338**
TENDL-2011	**2425**	**2429**	**2419**	**2431**	**2429**	**2428**	**2428**	**574**	**2416**
TENDL-2010	**2394**	**1157**	**1159**	**1156**	**1159**	**1140**	**1152**	**529**	**1086**
TENDL-2009	**2375**	**1163**	**1164**	**1116**	**1163**	**1127**	**1165**	**509**	**1141**
TENDL-2008	348	344	336	339	342	338	327		**342**
(JEFF-3.2)	*472*								*218*
(ENDF/B-VII.1)	*423*	*47*	*5*	*3*		2	*163*	*80*	*146*
(JENDL-4.0)	*406*								*90*

From: Dimitri Rochman

Photonuclear data libraries

	# nuclides	Contents	Comments
BOFOD (Russia)	9	Main xs channels and spectra	Actinides, basis for IAEA library
CNDC (China)	24	All xs channels and spectra	Basis for IAEA library
ENDFB7.1	164	MF3,6/MT5	Adopted IAEA library
IAEA	165		Best selection from 5 libraries
JENDL-2004	69	MF3,6/MT5,201-207	
KAERI (Korea)	143	MF3,6/MT5	Basis for IAEA library
LANL	13	MF3,6/MT5	Basis for IAEA library
TENDL-2017	2808	All xs, spectra and covariance data	

Models for TENDL-2017

- Optical model:
  - (Near)spherical: KD03 OMP
  - Rotational non-actinides: KD03 with reduction of imaginary potential
  - Actinides: Soukhovitskii global OMP
- Level densities:
  - Constant Temperature or Back-shifted Fermi Gas with KHG08 parameterization
- Photons:
  - Kopecky-Uhl Generalized Lorentzian
  - Quasi-deuteron of Chadwick et al
- Pre-equilibrium:
  - Two-component exciton model with KD05 parameterization
- Fission:
  - Multi-barrier Hill-Wheeler model

TENDL-2017: photonuclear data library

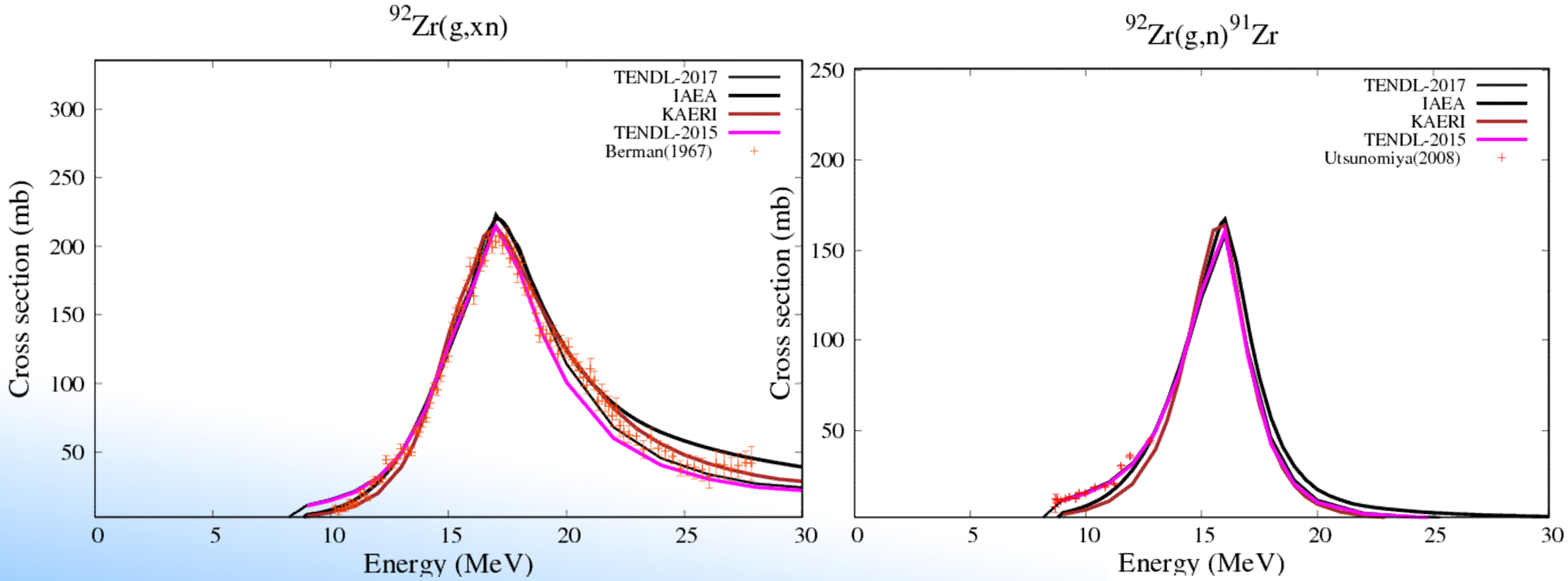
162 nuclides with experimental photonuclear data.

Three categories:

- Perfect “blind” fit (not surprising, we re-insert the GDR parameters)
- Problematic for TALYS: light nuclides
- Better description after adjustment of GDR parameters
  - 50 nuclides
  - Only E1 parameters were adjusted
  - In 80% of cases: adjustment of energy and strength of GDR by less that 5%.

Good but conflicting fits: ^{92}Zr

- All libraries rather good
- Which low-E tail is good?



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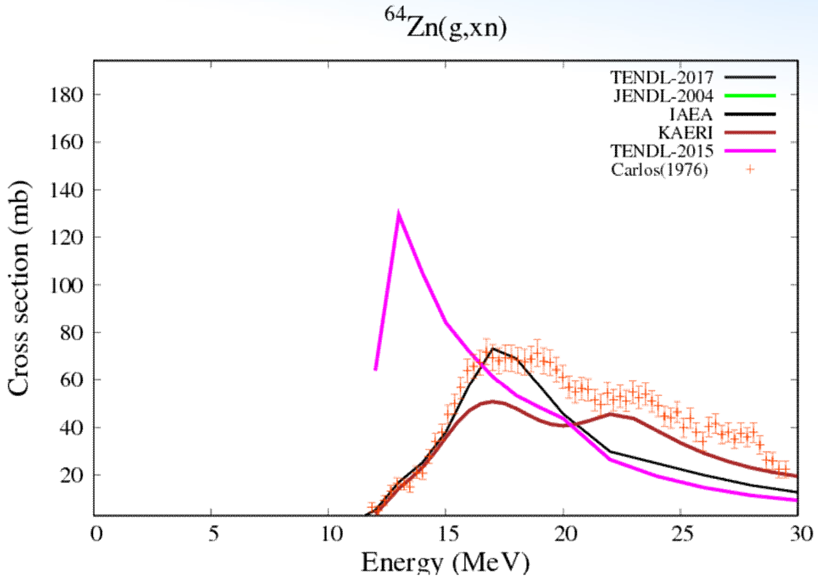
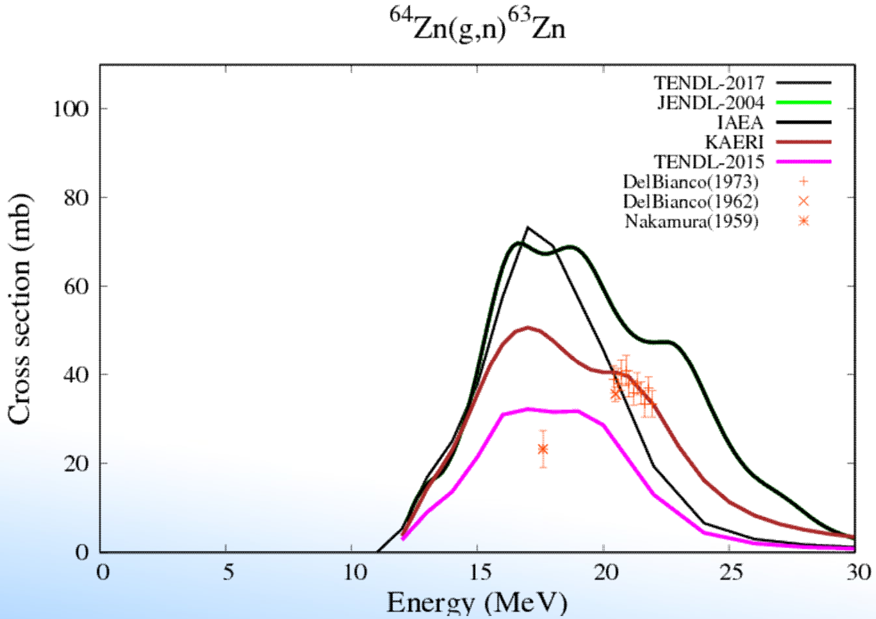
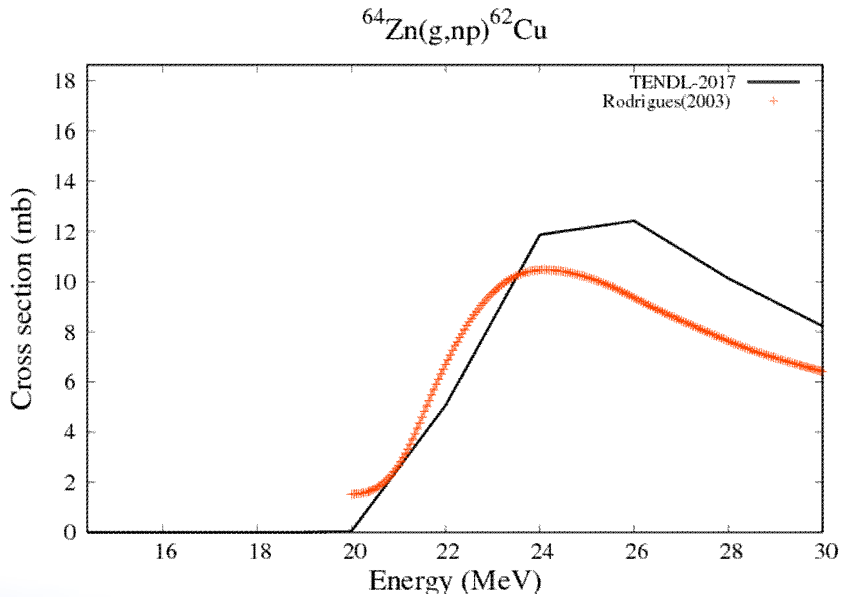
Improvement: ^{64}Zn

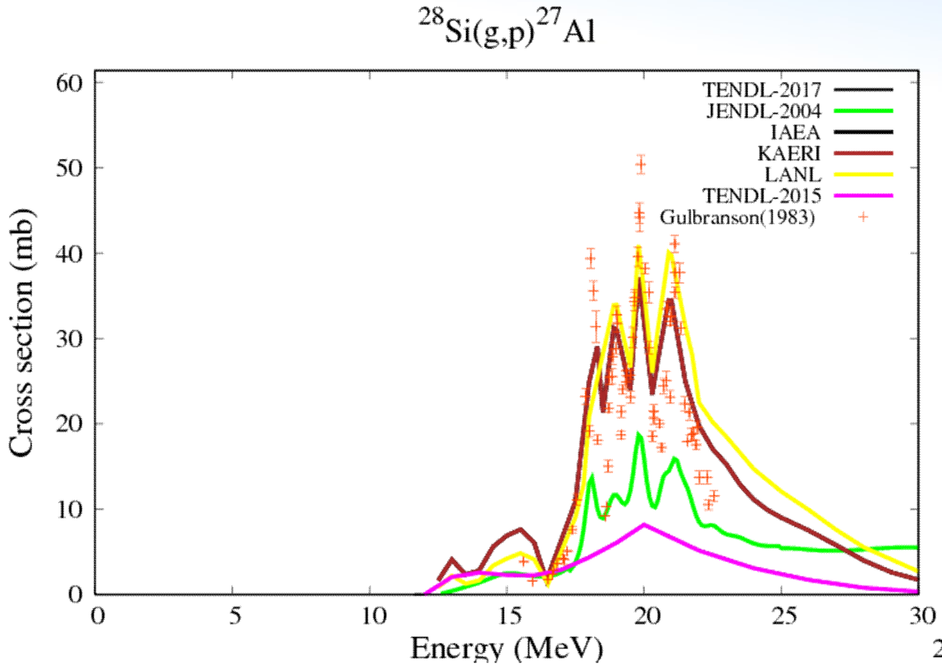


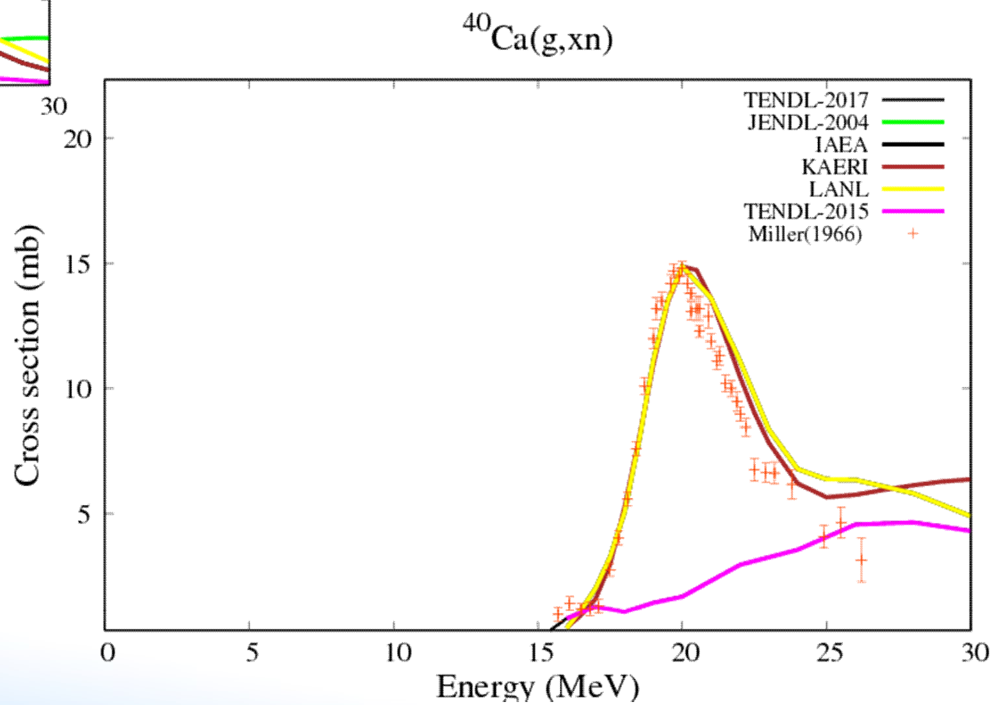
- TENDL-2015 contains computational error for 70 reaction channels
- TENDL predicts all channels



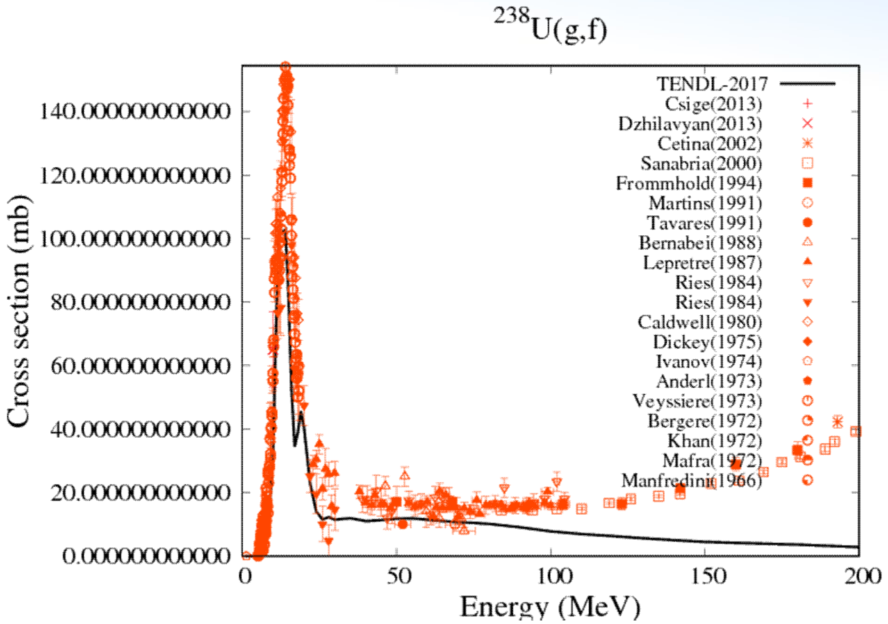


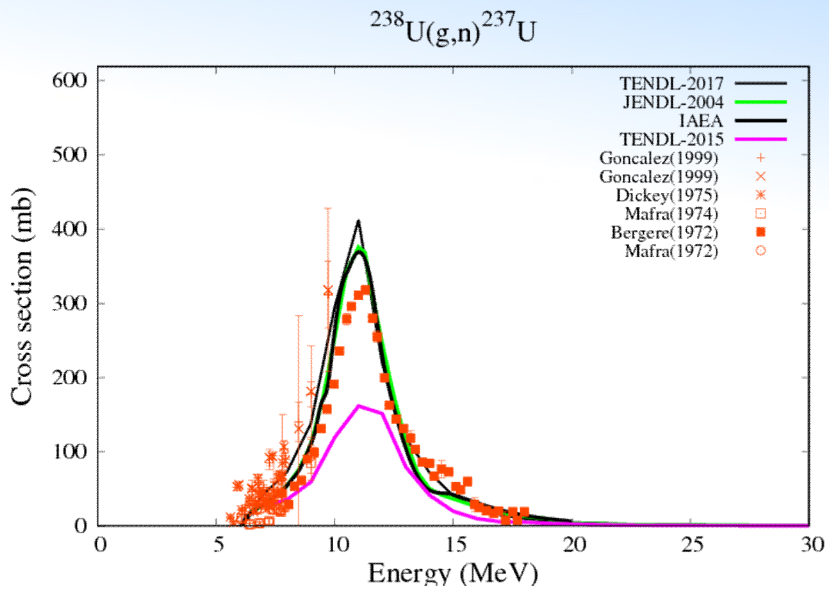
A < 40: trouble for TENDL

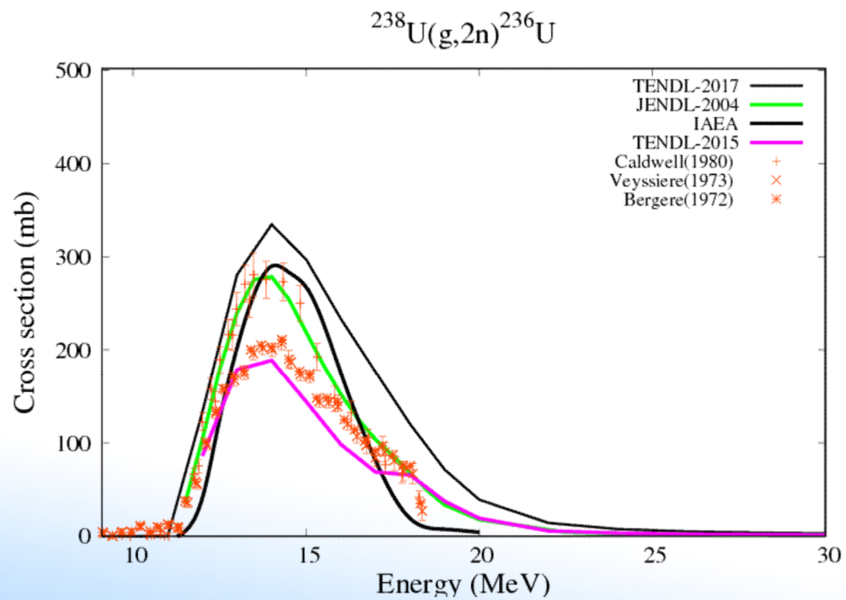




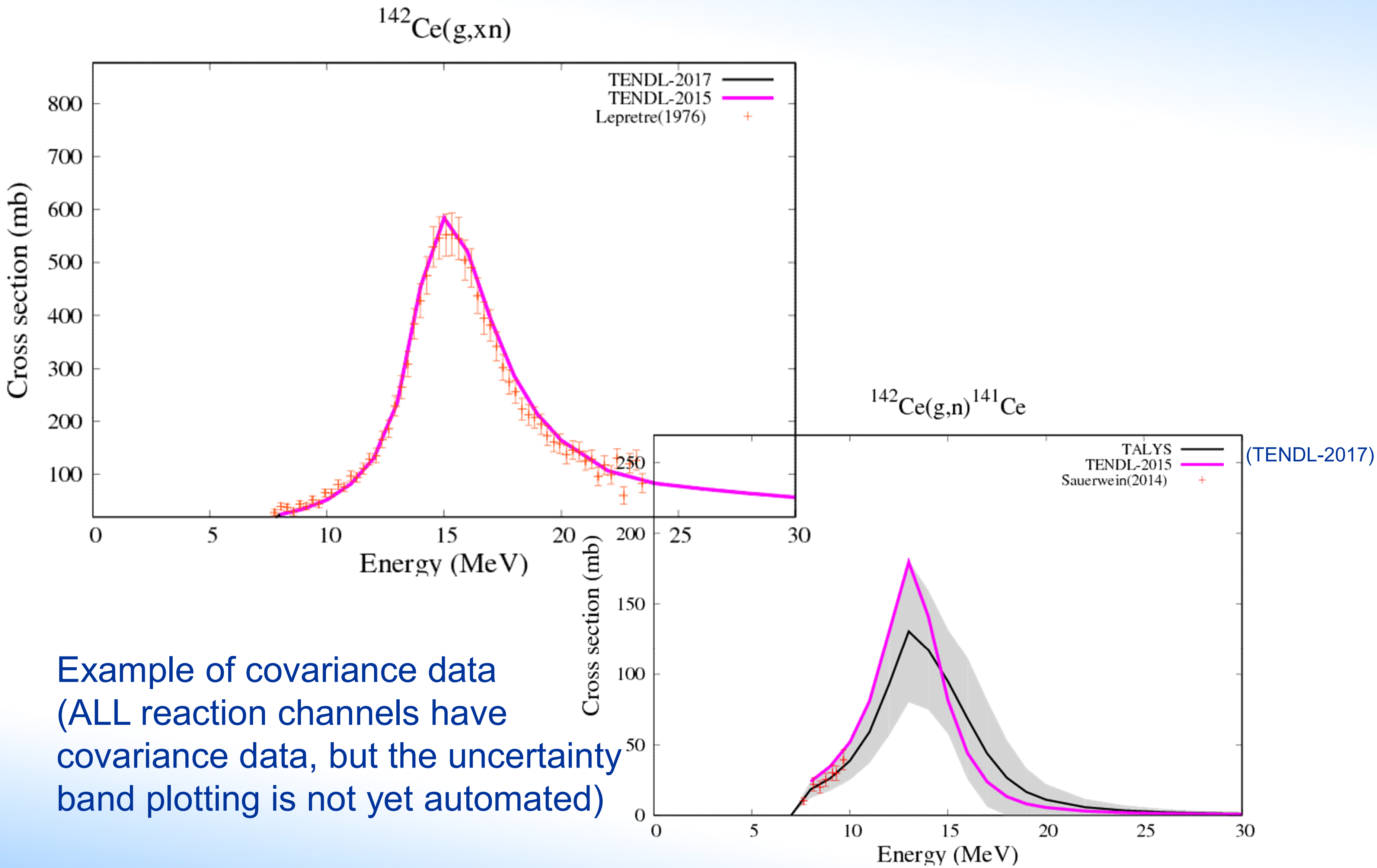
Actinides: photofission







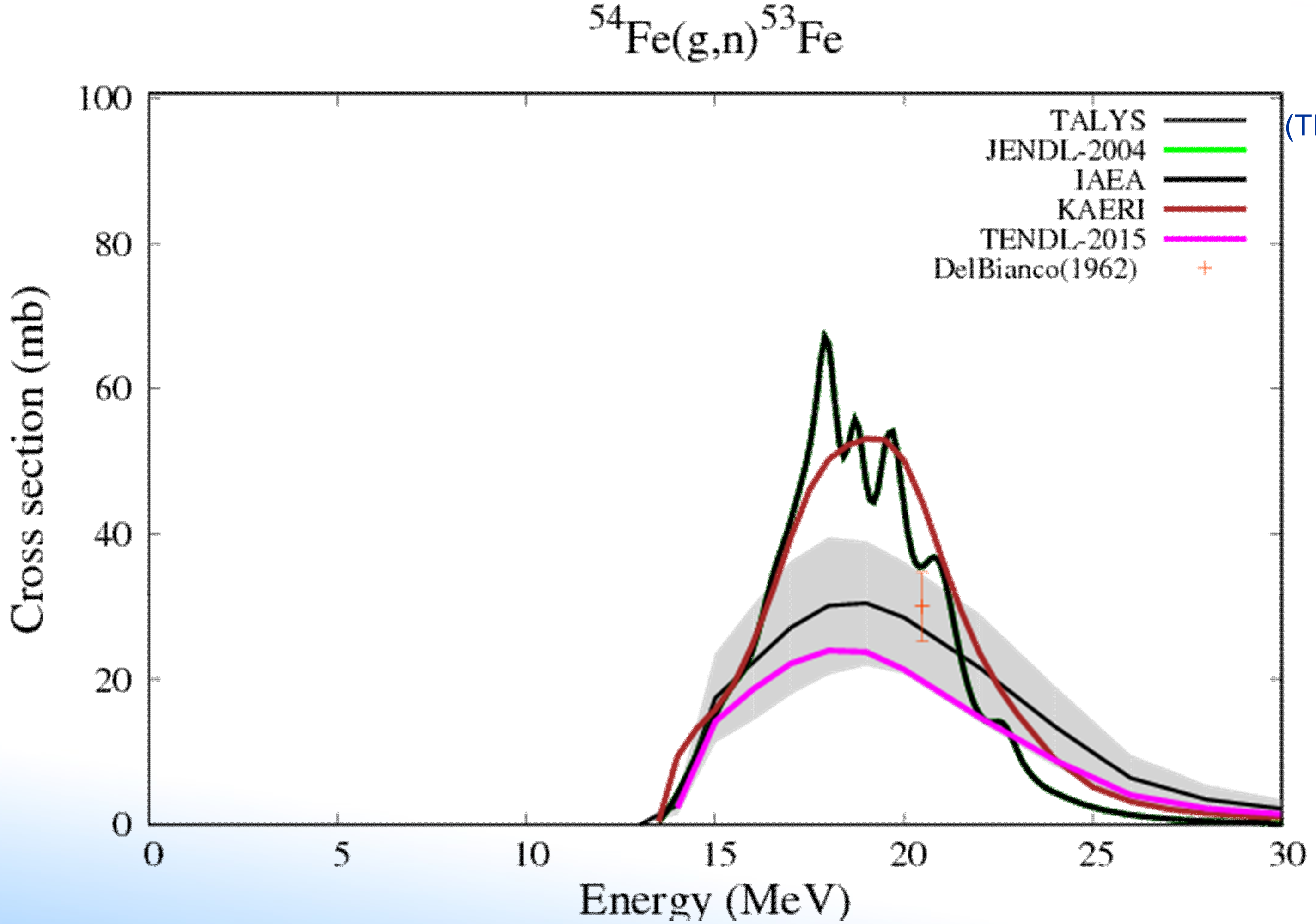
^{142}Ce: nothing but TENDL



Example of covariance data (ALL reaction channels have covariance data, but the uncertainty band plotting is not yet automated)

^{54}Fe: improvement

- Example of covariance data



(TENDL-2017)

Phenomenological vs microscopical

Practical experience:

- Optical model (KD03 OMP vs. JLM)
- Fission (Hill-Wheeler vs WKB + HFB)
- Level densities (Fermi gas vs. HFB combinatorial)
- Photon strength functions

  (Lorentzians vs. e.g. QRPA/D1M) (Goriely)

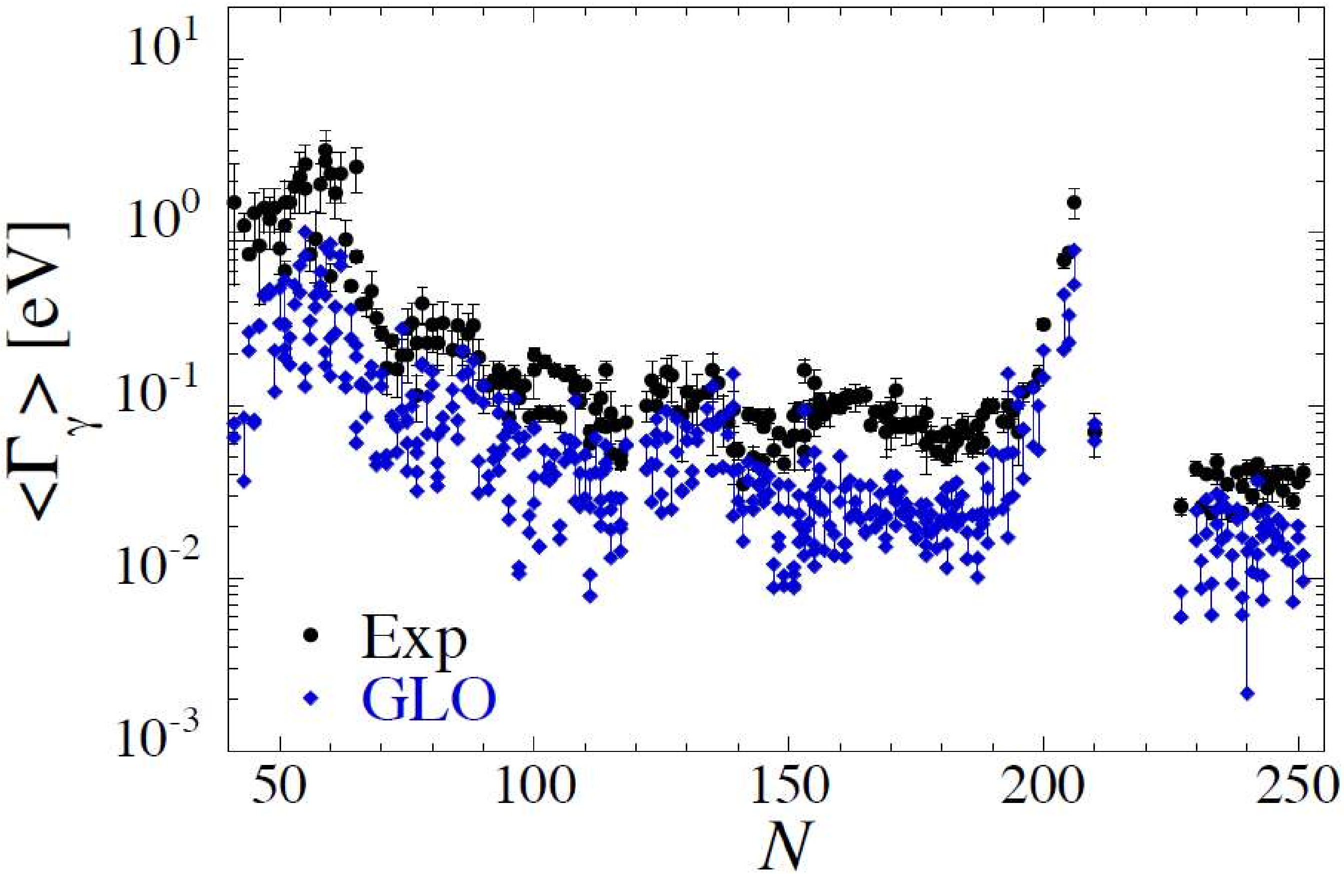
RELIABILITY

What helps: A relatively smaller number of reaction channels are sensitive to PSF, most notably (n,γ) and (γ,n) : phenomenological adjustments to PSF parameters affect no other channels (unlike OMP, level density)

GLO strength (E1 & M1) and its impact on the radiative width $<\Gamma_\gamma>$

$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$

Long-standing problem of the underestimate of $<\Gamma_\gamma>$ by Lorentzian-type models

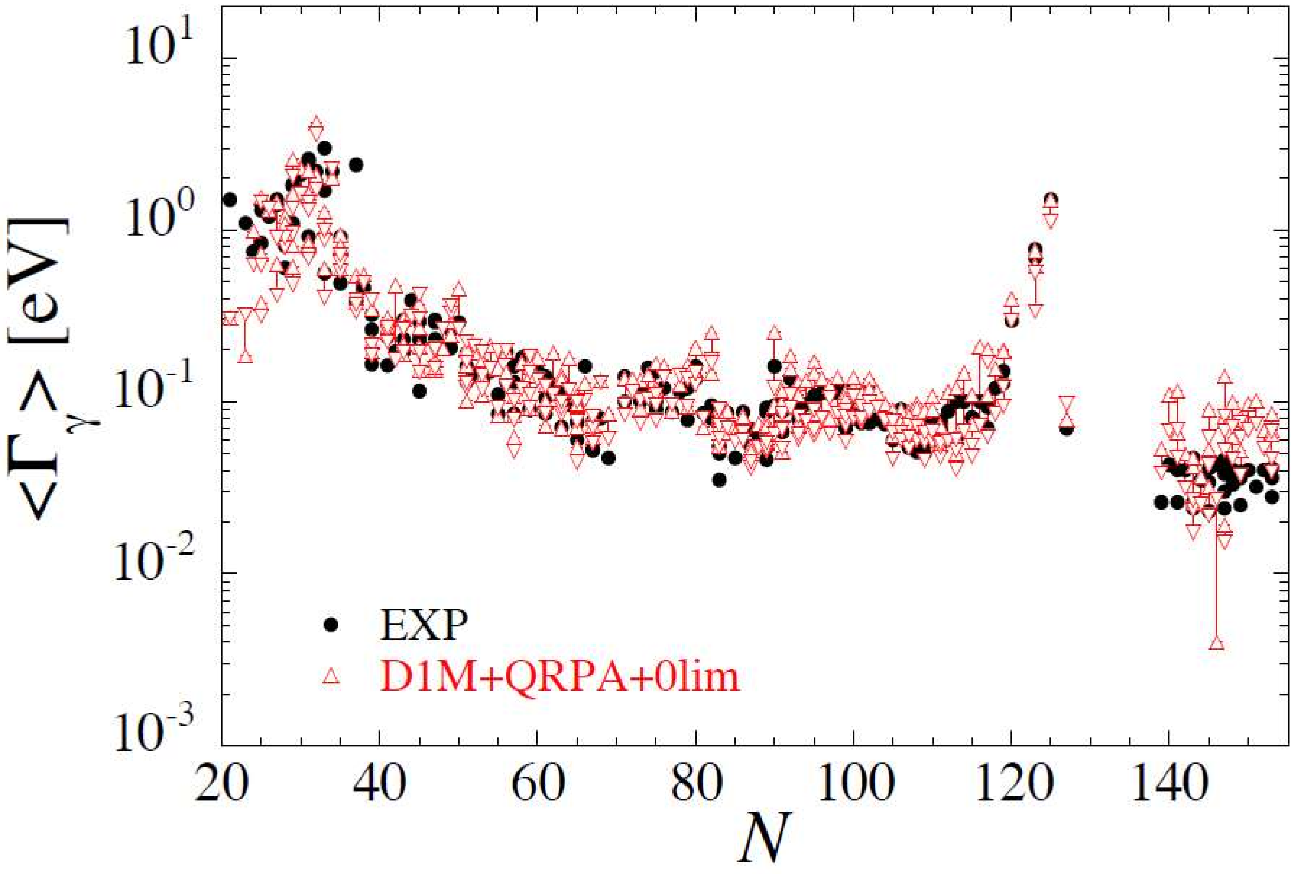


From Stephane Goriely

where error bars on predictions are obtained with different NLD models

D1M+QRPA E1 & M1 strength + non-zero limit and its impact on the radiative width $<\Gamma_\gamma>$

$$\langle\Gamma_\gamma\rangle = \frac{D_0}{2\pi}\sum_{X,L,J,\pi}\int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma)\times\rho(S_n+E_n-\varepsilon_\gamma,J,\pi)d\varepsilon_\gamma$$



From Stephane Goriely

where error bars on predictions are obtained with different NLD models

Summary photonuclear data library I

- The TENDL photonuclear data library is no longer "blind":
  - Reactions channels for 50 nuclides were fitted with TALYS, leading to TENDL-2017 photonuclear data library
  - Adjusted TALYS input files are 'frozen' as starting point for TENDL-2018,2019
  - Completeness, also with comparison to other libraries, is under control: nuclides, reaction channels, spectra, isomer production, 200 MeV, covariances, etc.
  - Underperformance of TENDL-2017:
    - Light nuclides (A < 40), other libraries, esp. KAERI library, do better IF there is experimental data
    - A few remaining individual channels for A > 40, where KAERI library gives better fits
  - TENDL-2017 will be available at the end of 2017.

Summary photonuclear data library II

- Microscopic QRPA + D1M photon strength functions with two adjustable TALYS parameters (‘etable’ and ‘ftable’) are expected to give superior results. This insight (and/or appetite) came too late for TENDL-2017.
  - More consistency of PSF’s for (n,γ) and (γ,n), which are so far not adopted universally in evaluation work.
  - One consistent choice for M1

- It would be a major motivation for evaluators if someone (and more than one!) would actually USE these data in nuclear technology. Several software packages (e.g. MCNP, FISPACT-II) are ready for this.

Thermal capture cross sections

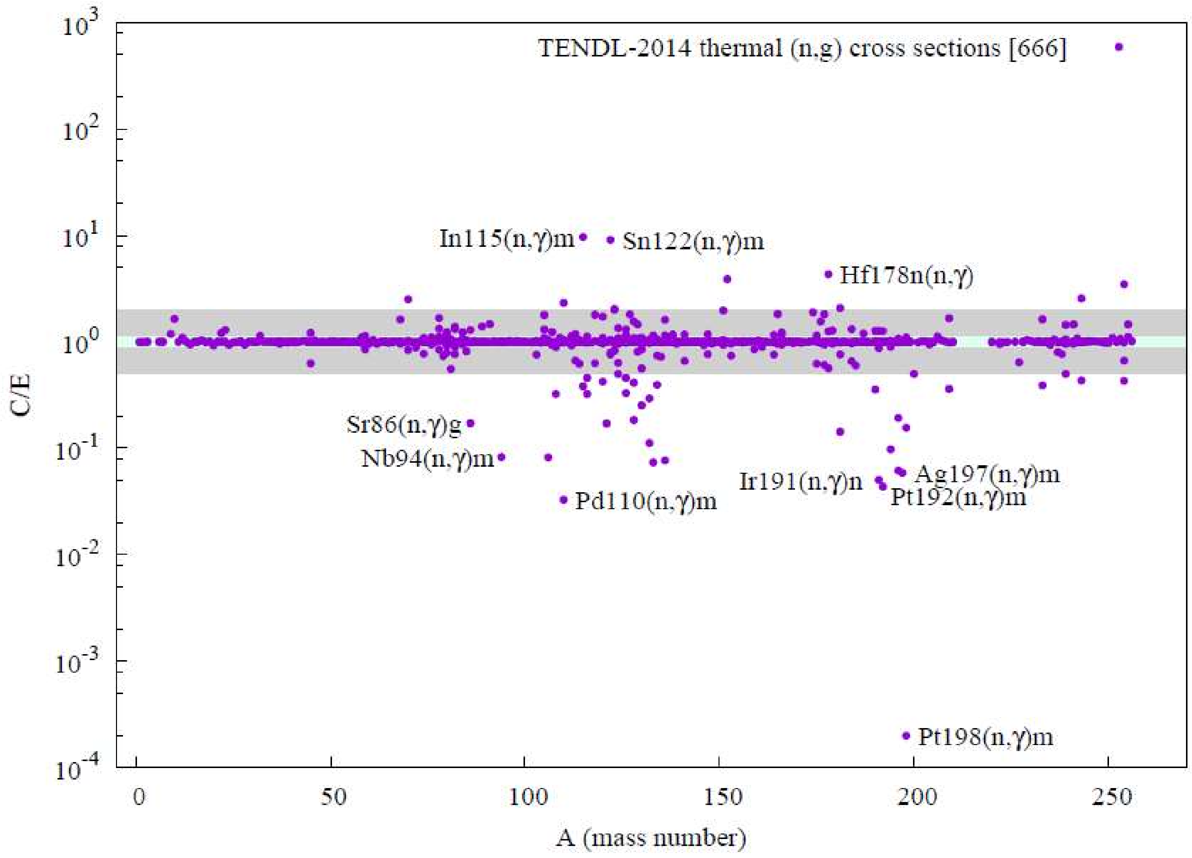


Figure 4: Distribution of TENDL-2014 (n,γ) thermal cross section C/E values against number of nucleons A. The bands represent regions of $\frac{1}{2}$<C/E<2 and |C-E|/E <10%.

Fleming et al, Probing experimental & systematic trends of the neutron -induced TENDL-2014 nuclear data library, UKAEA-R(15)30

Thermal (n,alpha) cross sections

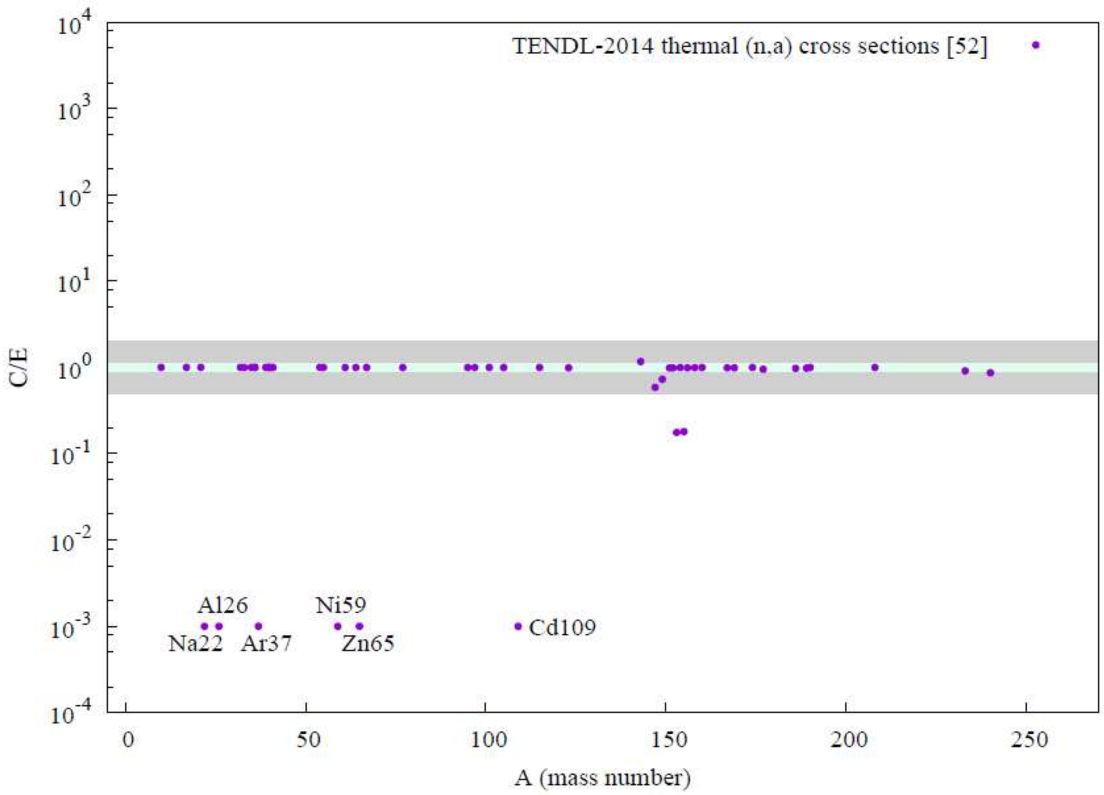


Figure 11: Distribution of TENDL-2014 (n,α) thermal cross section C/E values against number of nucleons A. The bands represent regions of $\frac{1}{2}$<C/E<2 and |C-E|/E <10%.

Fleming et al, Probing experimental & systematic trends of the neutron -induced TENDL-2014 nuclear data library, UKAEA-R(15)30

Maxw. Av. capture cross sections

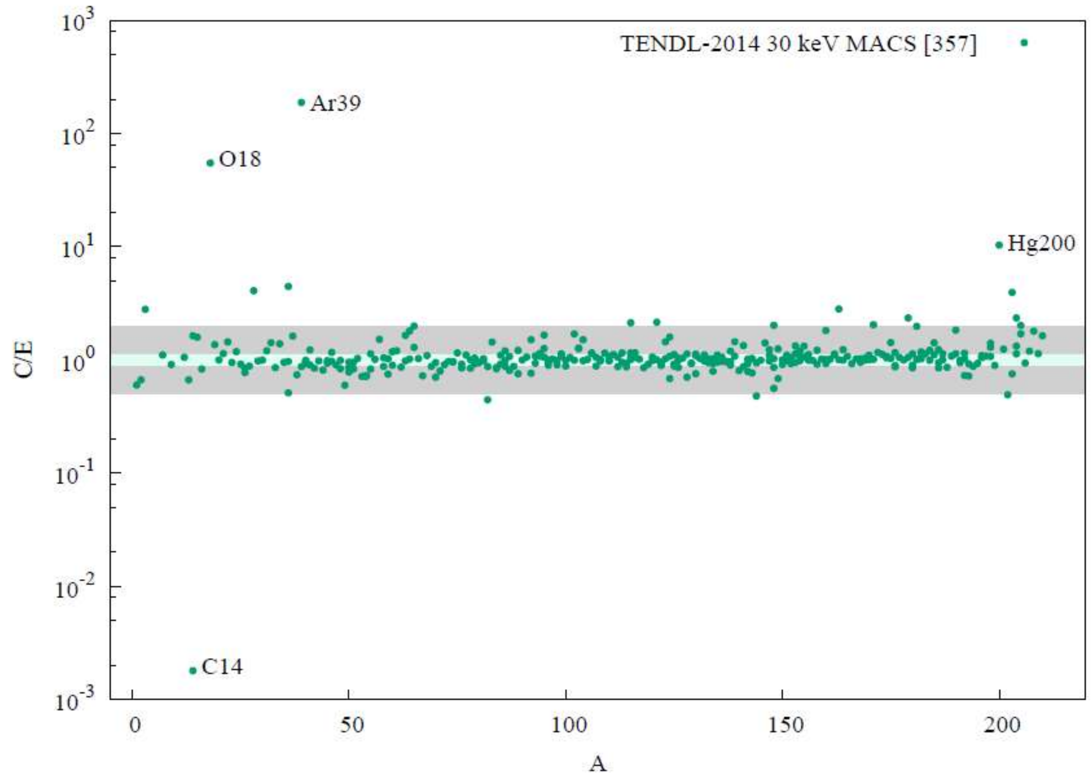


Figure 8: Comparison of all 357 KADoNiS 30 keV cross sections with TENDL-2014 values calculated with maxwav. A few nuclides are isolated which require an adjustment of over one order of magnitude. The bands represent regions of $\frac{1}{2}<C/E<2$ and $|C-E|/E < 10\%$.

Fleming et al, Probing experimental & systematic trends of the neutron -induced TENDL-2014 nuclear data library, UKAEA-R(15)30

MACS comparison with other libraries

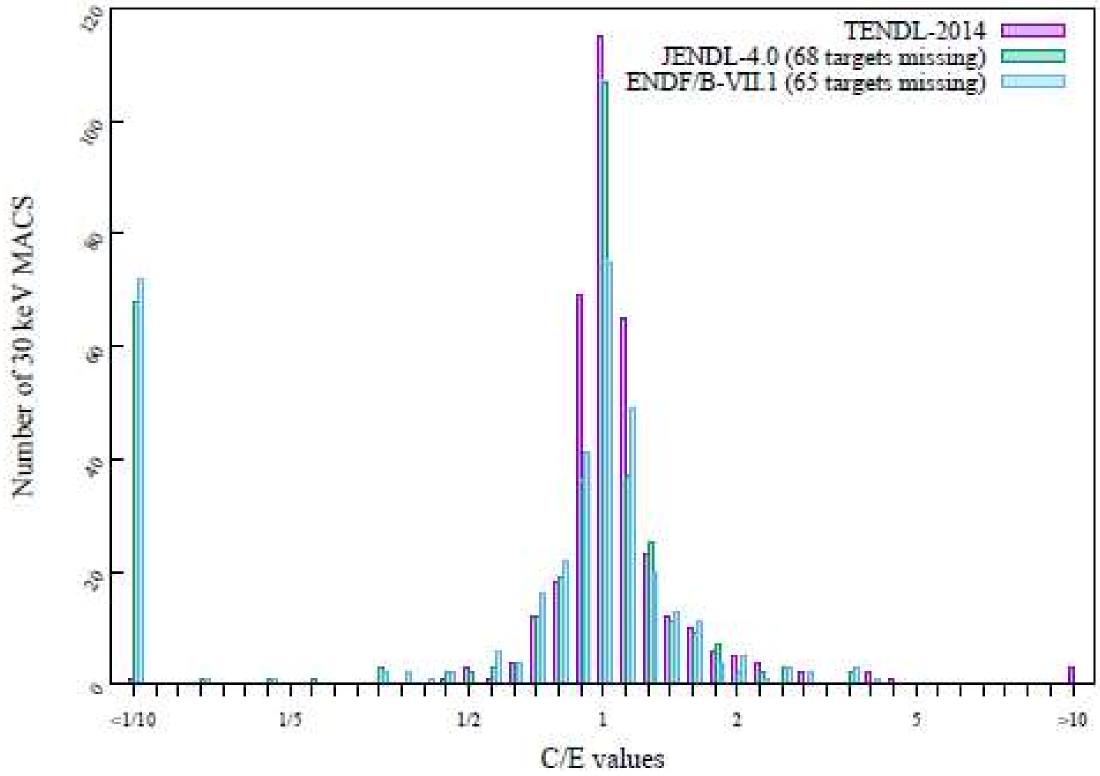
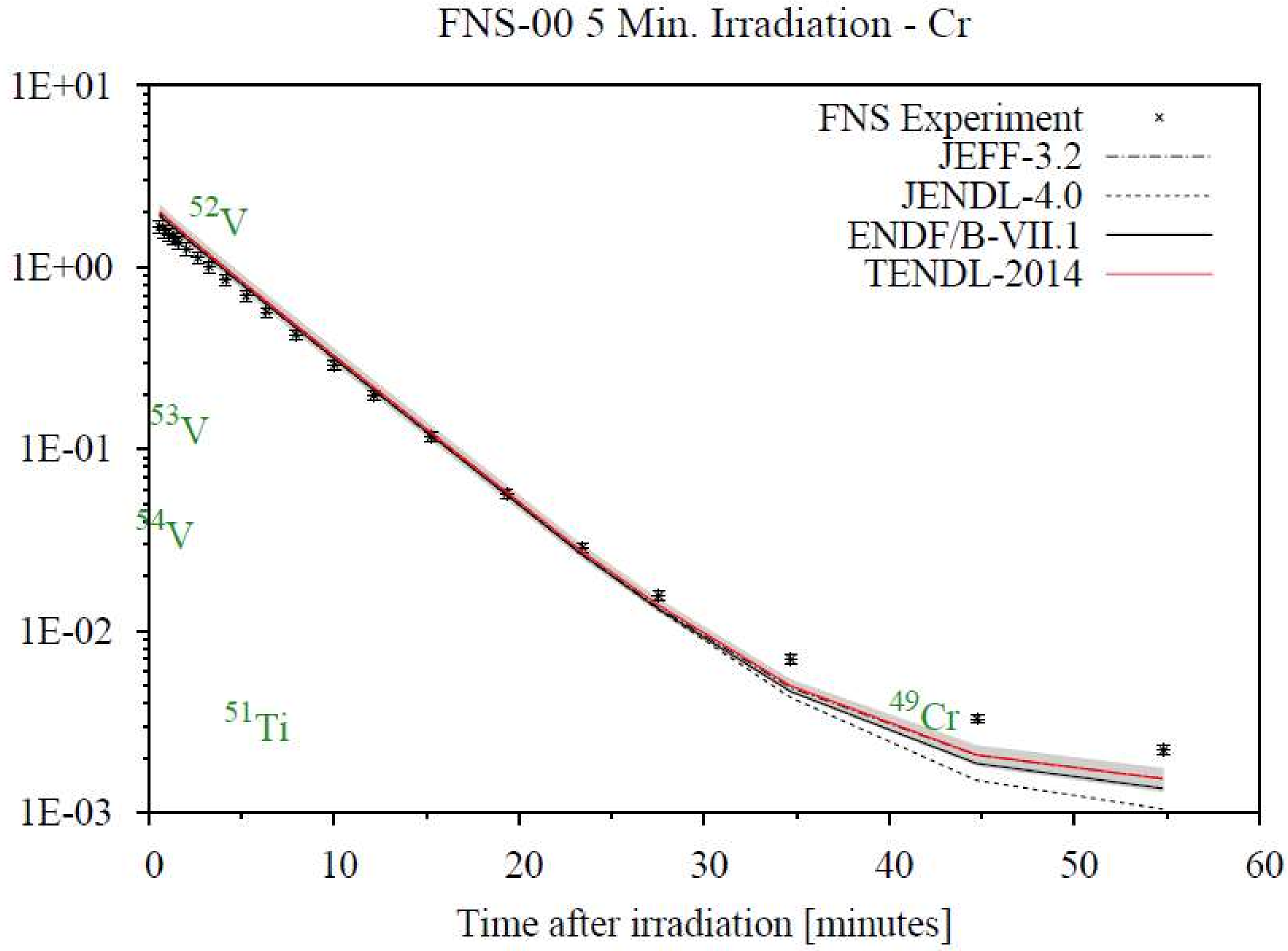


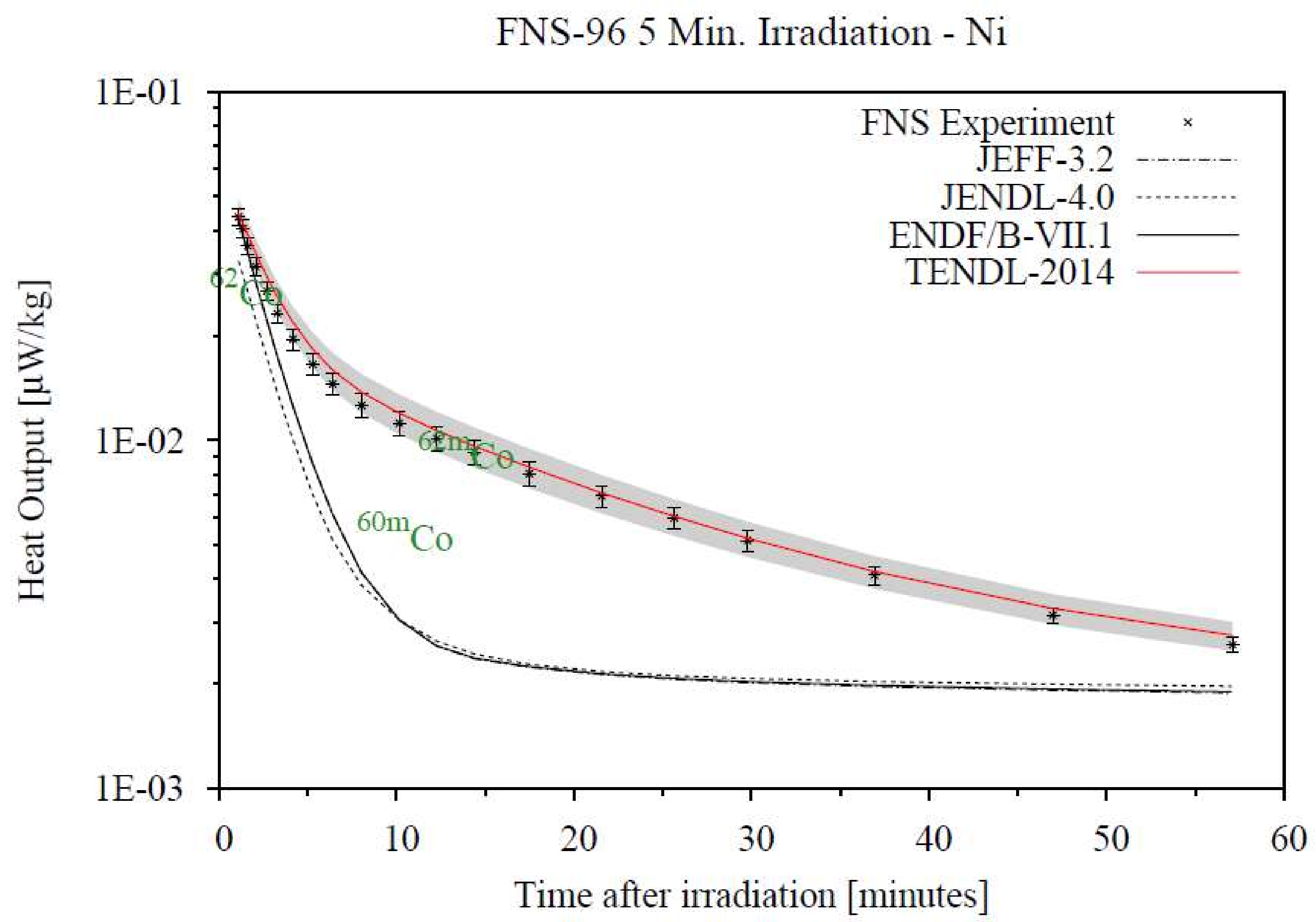
Figure 8: Comparison of C/E distributions overal all 357 KADoNiS 30 keV cross sections with TENDL-2014, JENDL-4.0 and ENDF/B-VII.1 values calculated with maxwav. C/E values for missing nuclides in JENDL-4.0 and ENDF/B-VII.1 are tallied in the <1/10 bin.

Sublet and Fleming, Maxwellian-averaged neutron-induced cross sections for kT=1 keV to 100 keV KADoNiS, TENDL-2014, ENDF/B-VII.1 and JENDL-4.0u nuclear data libraries UKAEA-R(15)29

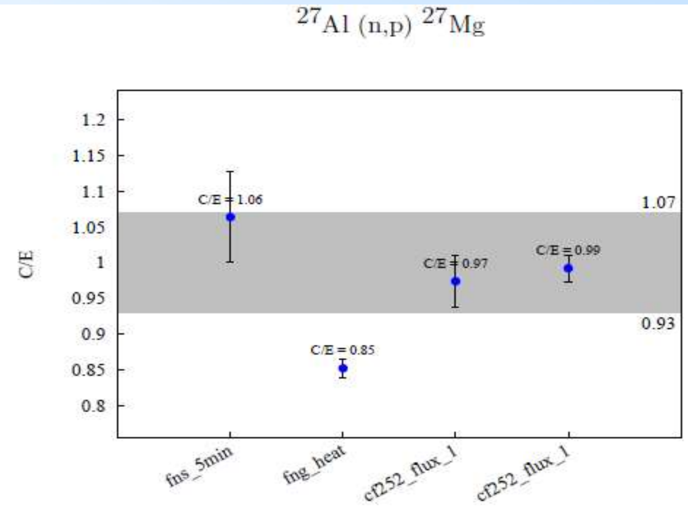
Chromium

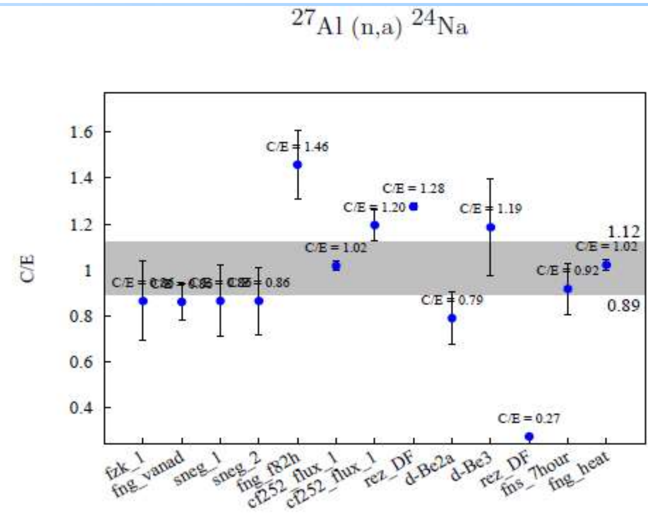


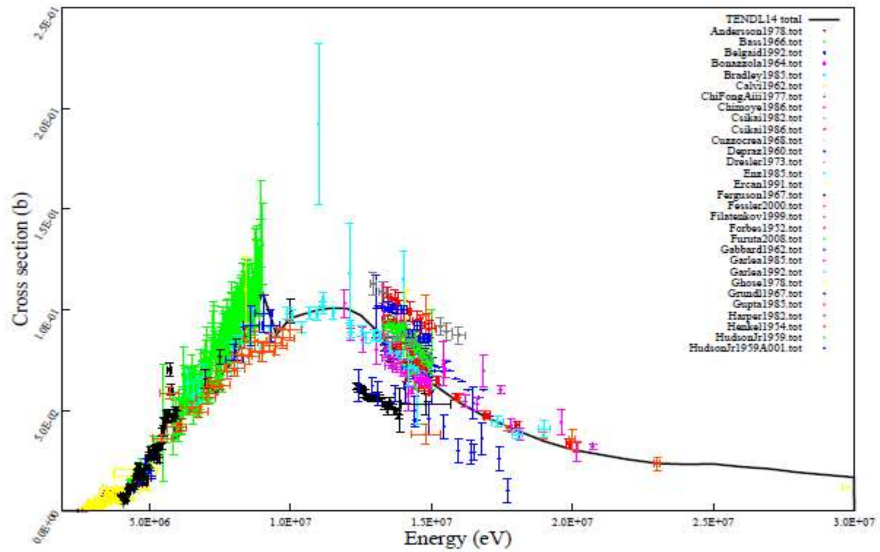
J.C. Sublet and M. Gilbert, Decay heat validation CCFE-R(15)25, january 2015

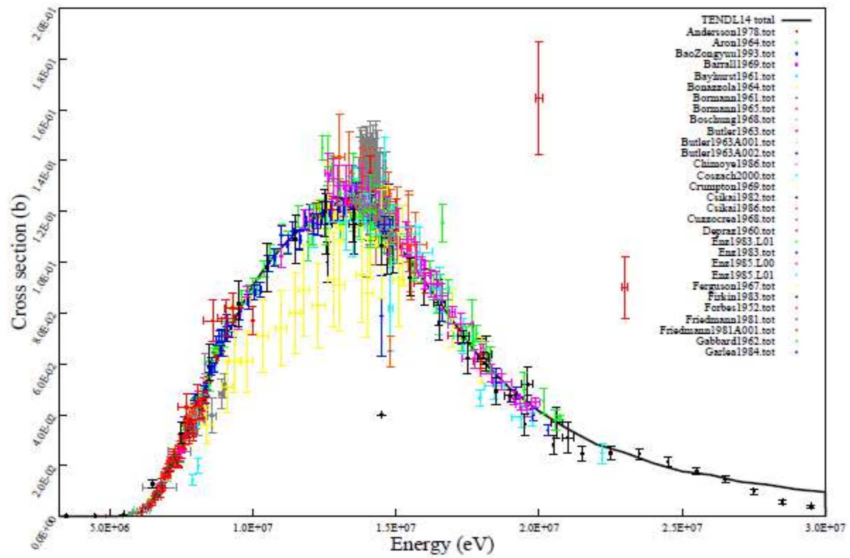


Decay heat should only be analyzed with General Purpose Libraries









M. Fleming, J.C. Sublet, J. Kopecky: Integro-differential validation, CCFE-R(15)27, March 2015

Next TALYS: 2017

- Release December 2017: TALYS-1.9
  - "Old-style" TALYS: leading release digit= 1
  - More flexibility for M1 gamma-ray strength functions
  - Implemented Kalbach's published model for break-up reactions
  - Broadening of resonance reactions for astrophysical reaction rates
  - Usual bug fixing and code cleaning

Next TENDL: 2017

- December 2017: Release of TENDL-2017
  - Neutrons:
    - Improvement of cross section values by Natalia Dzysiuk for fusion and fission product nuclides
    - General improvement of resonance parameters by Dimitri Rochman
    - Last (?) remaining ENDF format deficiencies removed
  - Photons:
    - Adjustment of TALYS parameters to experimental data
  - Protons, deuterons, tritons, He-3, alpha particles:
    - ENDF format completion for recoils

Next TALYS: 2018-2019

- TALYS-2.0
  - Full Fortran-95
  - TEFAL code included:
    - Complete ENDF formatting
    - Allows TALYS users to create ENDF data libraries
  - TASMAN code included:
    - Uncertainties, covariances, sensitivity profiles, Bayesian Monte Carlo, Total Monte Carlo
    - Allows TALYS users to perform uncertainty analyses, random nuclear data libraries and covariance evaluations
  - Opens up TENDL-like production to the entire world

Next TENDL: 2018

- Produced with TALYS-2.0
- Correct remaining deficiencies:
  - (n,p) and (n,alpha) resonances for low-energy positive Q-value reactions
  - Isomeric ratio for thermal (n,gamma) reactions
- Systematic validation scheme:
  - CCFE: Integral activation measurements, decay heat, radiation damage, etc. (Fleming, Gilbert et al.)
  - NRG: van der Marck criticality (ICSBEP) and shielding (SINBAD) benchmarking suite
  - PSI: EXFOR, thermal, MACS and resonance validation, library optimization with the “Petten method”, FPY (Rochman)
  - IAEA: “EASY-database”, processing, all non-criticality validation (Sublet), criticality (Trkov), differential (EXFOR) validation (Koning)
  - Try to minimize the turnaround time. Ideally: integral testing during evaluation
- TENDL paper in Nuclear Data Sheets, January 2019.

Beyond TALYS-2.0: 2019 - 2022

IAEA 60 Years Atoms for Peace and Development

- Communication:
  - New Tutorial with “everything”:
    - All physics of the “Old” TALYS manual
    - All ENDF-6 formatting (TEFAL)
    - All Monte Carlo, covariance etc. (TASMAN)
    - Guide to TENDL production and Total Monte Carlo
    - Sample cases throughout the tutorial
    - Acknowledge ALL TALYS use throughout the tutorial (very challenging
  - Youtube video for installation, basic use, possibilities etc.
  - Courses: Ready-to-use material for e.g. 4-hour, 16-hour and 40 hour course

Beyond TALYS-2.0: 2019 - 2022

- Code:
  - Further modernization
    - Even more modular and memory efficient
  - Remaining physics:
    - Stable and robust FY prediction
    - Nubar
    - PFNS
  - Enable full particle evaporation up to 1 GeV
  - Complete adoption of resonance parameters
- Not on the radar yet:
  - Heavy-ion reactions
  - Light nuclides

Beyond TENDL-2018: 2019-2022

- Competing with other libraries on nominal values
- Libraries for all particles come with covariance data and many random files
- Up to 1 GeV
- Couple TENDL to web-based medical isotope production App
- New things we think of in 2018

60 Years

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Thank you!