

## **TALYS and TENDL: status and future**

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### Contents



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





A nuclear reaction program





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**



#### 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, g 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



#### Microscopic / Phenomenologic



#### Microscopie / Phenomenologic

Atoms for Peace and Development

60 Years

IAEA



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



TALYS: <sup>°°</sup>Y(n,γ)



#### **Simulated resonances**



- Alternative approach to the HF calculations: the High Fidelity Resonance calculations (HFR)
- Presented in <u>ANE 50 (2013) 60</u>
  - 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  $D_0$ ,  $\Gamma_\gamma$ ,  $\Gamma_n$ ,  $\Gamma_f$ ... 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





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



60 Years IAEA Atoms for Peace and Development

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



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

## **TENDL** philosophy



- 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 | Deuterion | Triton | Apple | Heliuns | Photon | Fi. Viela | Corariance |  |
|----------------|---------|--------|-----------|--------|-------|---------|--------|-----------|------------|--|
| 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<br>and spectra     | Actinides, basis for IAEA library |
| CNDC (China)   | 24         | All xs channels and spectra         | Basis for IAEA<br>library         |
| ENDFB7.1       | 164        | MF3,6/MT5                           | Adopted IAEA<br>library           |
| IAEA           | 165        |                                     | Best selection from 5 libraries   |
| JENDL-2004     | 69         | MF3,6/MT5,201-<br>207               |                                   |
| KAERI (Korea)  | 143        | MF3,6/MT5                           | Basis for IAEA<br>library         |
| LANL           | 13         | MF3,6/MT5                           | Basis for IAEA<br>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: <sup>92</sup>Zr



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



### Improvement: <sup>64</sup>Zn















Example of covariance data



### Phenomenological vs microscopical

R E

Α

В

#### 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)

What helps: A relatively smaller number of reaction channels are sensitive to PSF, most notably  $(n,\gamma)$  and  $(\gamma,n)$ : phenomenological adjustments to PSF parameters affect no other channels (unlike OMP, level density) GLO strength (E1 & M1) and its impact on the radiative width  $\langle \Gamma_{\gamma} \rangle$ 

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

Long-standing problem of the underestimate of  $\langle \Gamma_{\gamma} \rangle$  by Lorentzian-type models



where error bars on predictions are obtained with different NLD models



where error bars on predictions are obtained with different NLD models

# Summary photonuclear data library

- 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  $(n,\gamma)$  and  $(\gamma,n)$ , 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 Years



Figure 4: Distribution of TENDL-2014 (n, $\gamma$ ) 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, $\alpha$ ) 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 and Development



Figure 8: Comparison of all 357 KADoNiS 30 keV cross sections with TENDL-2014 values calculated with maxway. 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 maxway. 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





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

- 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, 16hour 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



# Thank you!

