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TALYS-1.0

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Abstract. TALYS is software that simulates nuclear reactions which involve neutrons, gamma-rays, protons, deuterons, tritons, helions and alpha-particles, in the 1 keV–200 MeV energy range. A suite of nuclear reaction models has been implemented into a single code system, enabling us to evaluate basically all nuclear reactions beyond the resonance range. A short overview is given of the main nuclear models used. The predictive power of the code is illustrated by comparing calculated results with a few sets of experimental observables. Our aim is to show that TALYS represents a robust computational approach that covers the whole path from fundamental nuclear reaction models to the creation of complete data libraries for nuclear applications. All further info on TALYS is available on the website www.talys.eu. As an important applied example we present SALTY, a nuclear data library for all projectiles, target nuclides and energies in both tabular and ENDF-6 format, that is based entirely on the TALYS nuclear model code.

1 Introduction

At ND-2004, the beta version of the TALYS code (version 0.64) was released. TALYS is developed at NRG Petten, the Netherlands and CEA Bruyères-le-Châtel, France with the objective to provide a complete and accurate simulation of nuclear reactions in the 1 keV–200 MeV energy range, through an optimal combination of reliable nuclear models, flexibility and user-friendliness. Meanwhile, TALYS has enjoyed widespread use, mainly for technological applications but also for fundamental research such as astrophysics and basic nuclear reaction and structure models. Feedback from users and an extensive validation scheme have allowed us to leave the beta testing stage and to release TALYS-1.0. A website with the full software package and a suite of validation reports is available at www.talys.eu. As usual, we have put a lot of emphasis on quality assurance procedures, including stability, robustness and validation of the code. Additions to the previous beta version include among others a larger variety of microscopic and phenomenological level density models, astrophysical reaction rates, better fission models and preparation of the code for covariance calculations.

The importance of nuclear model codes in contemporary nuclear data evaluation will be addressed in another contribution to this conference [1]. Here, we just mention that the global use of TALYS is divided roughly in two: (a) as a nuclear physics tool for the analysis of experiments and for associated academical and fundamental physics (e.g., astrophysics [2]) purposes; (b) as a nuclear data tool to generate complete sets of data, in e.g., ENDF-6 format, for technological applications such as conventional and innovative power reactors (GEN-IV), accelerator applications and transmutation of radioactive waste, fusion reactors, homeland security, medical isotope production and radiotherapy, and oil-well logging.

For both fundamental and applicational use, there are two approaches possible with TALYS: (1) A very detailed study of one or a few nuclear reactions, possibly including adjustment to experimental data with nuclear model parameters, for e.g., a new measurement that reveals a new physical effect which can be modeled with the code, or the precise evaluation of all reactions for one particular isotope for e.g., the JEFF nuclear data library; (2) Massive default ("blind") calculations for hundreds or thousands of nuclides, for e.g., a large cross section database for astrophysical reaction rates, or thousands of complete ENDF-6 formatted data libraries, allowing transport and activation codes to always have a reasonably good answer.

The code comes with a large set of individual sample cases that addresses the precise reaction descriptions mentioned under (1). The release of TALYS-1.0 is also accompanied by a huge nuclear database, addressing (2).

2 Nuclear models

Since TALYS-0.64 was released at ND-2004, various extra features have been added to the code. Most of them will be explicitly mentioned below. Also, various publications are now available that give a detailed outline of the implemented physics [3]–[6]. The TALYS manual [7] is the most comprehensive source of information.

2.1 Nuclear structure and model parameters

All nuclear models make use of structure and model parameters, so there is an automatic reference to parameters as masses, resonances, discrete levels, etc. With a few exceptions, our database is based on the Reference Input Parameter Library [8].

2.2 Optical model and direct reaction model

We use the coupled-channels code ECIS-06 [9] as a subroutine for all optical model and direct reaction calculations. ECIS-06 delivers the basic observables such as the elastic

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angular distribution, the reaction and the total cross sections. Moreover it yields the transmission coefficients required for compound nucleus calculations and all cross sections and angular distributions for discrete states. The default optical model potentials (OMP) used in TALYS are the local and global parameterisations for neutrons and protons of ref. [10]. For nuclides outside the scope of this OMP, i.e., strongly deformed nuclides, we allow input of potentials on an individual basis. New in TALYS-1.0 is that the global deformed potential of ref. [11] is used as the default for actinides. With this scheme, coupled-channels calculations for various types of deformation (symmetric-rotational, harmonic-vibrational, vibration-rotational, and asymmetric-rotational) can be automatically performed. For near-spherical nuclides, direct reactions are calculated with DWBA, and inelastic scattering off odd-A nuclei is described by the weak-coupling model. Also, microscopic OMP calculations with the JLM method [12] can be performed. For deuteron, triton, helium-3 and alpha OMPs, we use a folding approach based on the aforementioned nucleon OMPs.

2.3 Compound nucleus model

Compound nucleus reactions are calculated with the Hauser-Feshbach formalism. For the first, binary interaction of the projectile and the nucleus, width fluctuation corrections (WFC) are included to account for the correlations that exist between the incident and outgoing waves. TALYS enables simulation with three different WFC expressions: the HRTW, Moldauer, and Gaussian Orthogonal Ensemble model, of which the Moldauer model has been established [13] as the best practical choice. All WFC models are generalized to include continuum particle emission, gamma-ray competition and fission. Gamma-ray coefficients are modeled with Kopecky-Uhl's generalized Lorentzian and the appropriate giant-dipole resonance parameters. A new option in TALYS-1.0 is the possibility to replace this by Hartree-Fock-Bogolyubov (HFB) based gamma ray strength functions from Goriely [14]. Besides cross sections, compound angular distributions are calculated using Blatt-Biedenharn coupling factors, again within a full Hauser-Feshbach expression with WFC. For multiple emission, the whole reaction chain is followed by depleting each continuum bin, under strict angular momentum and spin selection rules, with particle, gamma or fission decay until all channels are closed. In the process, all particle and residual production cross sections are accumulated to their final values. Non-equidistant emission energy grids in this decay scheme ensure enough precision in the compound evaporation peaks.

New in TALYS-1.0 is the ability to calculate astrophysical reaction rates [14]. For this, a loop over excited target states is made within the WFC compound nucleus model, after which the results are folded with a Maxwellian spectrum.

2.4 Level densities

TALYS-1.0 enables a choice between various level density models, such as the Constant Temperature Model (CTM), the Back-shifted Fermi Gas Model, and the Generalized Superfluid Model. The standard approach is a CTM fitted to the known discrete states, at low energy, and a Fermi gas model at high energies, with shell- and energy-dependent level density parameter a. For non-fissile nuclides, we often use an effective level density model, i.e., all collective enhancements are included in the level density parameter a. For fissile nuclides, we account for explicit rotational and vibrational enhancement as well as their appropriate damping at high energies. All level density parameterizations are directly derived from the latest collections of experimental discrete levels and mean resonance spacings [8].

An important new feature is the availability of parity-dependent HFB based level densities [15] in tabular form, enabling a direct study of the impact of such microscopical level densities on nuclear reaction yields.

2.5 Fission

For fission, the default model used in TALYS is based on the Hill-Wheeler expression for the transmission coefficient for one, two or three barriers. If the excitation energy of the compound nucleus is lower than the barrier heights, fission transmission coefficients display a resonant structure which is due to the presence of nuclear excited levels in the second well of the potential energy surface. These so-called class II states modify the fission transmission coefficients. The total fission transmission coefficient for a compound nucleus is then obtained by summing the individual Hill-Wheeler terms over all head band transition states and, for the continuum, integrating it using the aforementioned fission level densities. Multi-chance fission for all residual nuclides is included. A future development is to replace the simpler models by microscopic fission path predictions.

TALYS predicts fission yields. This is done with the multi-modal random neck rupture model and the scission point model.

2.6 Pre-equilibrium model

For energies above a few MeV, pre-equilibrium reactions play an important role. For nucleon reactions, we have implemented a two-component exciton model with a new form for the internal transition rates, which yields an improved description of pre-equilibrium processes over the whole energy range [16]. Another feature necessary to cover a large energy range is the generalization of multiple pre-equilibrium processes up to any order of particle emission. This is accomplished by keeping track of all successive particle-hole excitations of either proton or neutron type. Pre-equilibrium angular distributions are predicted by Kalbach's systematics.

On top of the contribution of the single-particle exciton model, which yields essentially structureless emission spectra, we add a contribution from giant resonances, computed with a macroscopic, phenomenological model, accounting for the energy weighted sum rule.

Pre-equilibrium photon emission is taken into account and for pre-equilibrium reactions involving deuterons up to alpha particles, breakup, stripping, pick-up and knock-out mechanisms are added through Kalbach's latest phenomenological model [17] (an upgrade of her older model used in TALYS-0.64), resulting in a much better prediction of complex particle cross sections as compared to many older reaction codes. However, the (very) phenomenological nature of the model still provides a challenge to construct a more physical approach for these reactions in the future.

3 Code construction, verification and validation

TALYS-1.0 is written in Fortran77, and so far has been successfully compiled and tested with many f77 and f90/f95 compilers. We have aimed at a setup that is as modular as Fortran77 allows it to be, using programming procedures that are consistent throughout the whole code. In total, there are about 270 subroutines adding up to a total of more than 42 000 lines, plus the 20 000 lines of the ECIS-06 subroutine. The code is rather flexible in its use, enabling "idiot-proof" 4-line input files, but also very specific reaction specifications, which can be constructed with the more than 200 keywords that are available. The code has been thoroughly tested on a formal level, through random input files (probing every corner of the code) and full dripline-to-dripline calculations have been performed to validate the code computationally and to test the continuity (smoothness) of the results.

The following data can be calculated:

- Total, elastic and reaction cross sections,
- Non-elastic cross sections per discrete state,
- Elastic and non-elastic angular distributions,
- Exclusive reaction channels ((n,2n), (n,np), etc.),
- Exclusive double-differential spectra,
- Exclusive isomeric production cross sections,
- Discrete and continuum gamma-ray production cross sections,
- Extrapolation of non-threshold cross section down to the thermal energy range [18],
- Total particle production cross sections, e.g., (n,xn),
- Single- and double-differential particle spectra,
- Residual production cross sections (+ isomers),
- Level density tables,
- Astrophysical reaction rates,
- Recoils,
- Fission cross sections and fission yields.

To illustrate some possibilities of TALYS, we give 2 entirely different examples. In figure 1 we compare TALYS with experimental data and several nuclear data libraries for neutron-induced fission on ^{241}Am. Very detailed nuclear models and associated parameterizations lie at the basis of this result. A detailed dispersive deformed optical model was constructed [19], and various level density parameters and fission barrier parameters were adjusted to obtain this fit, as well as equally good fits in the competing reaction channels (not shown here). Even with a flexible nuclear model code, it requires weeks/months of work to obtain a good reaction description of just one actinide. In addition, the modeling is of a highly phenomenological nature (about 10–20 adjustable parameters), which is unavoidable as long as the required breakthrough in fission reaction modeling has not been realized. Figure 2 shows another extreme of TALYS usage. To test our level density models [20], a comparison has been made between default ("blind") TALYS calculations and all

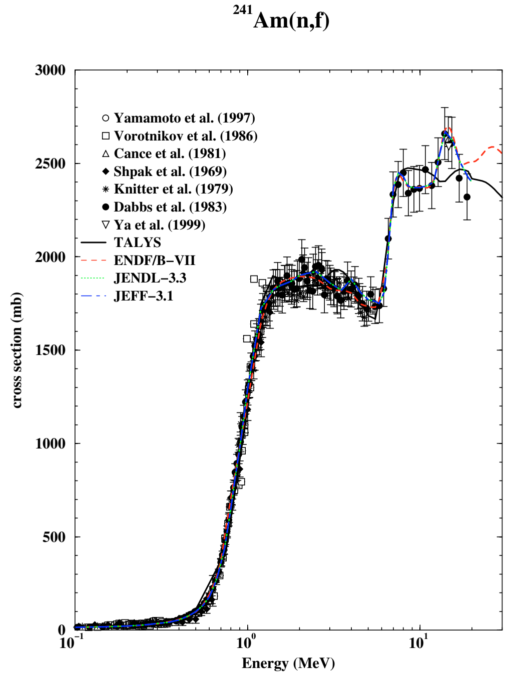

Fig. 1. Neutron-induced fission cross section for ^{241}Am.

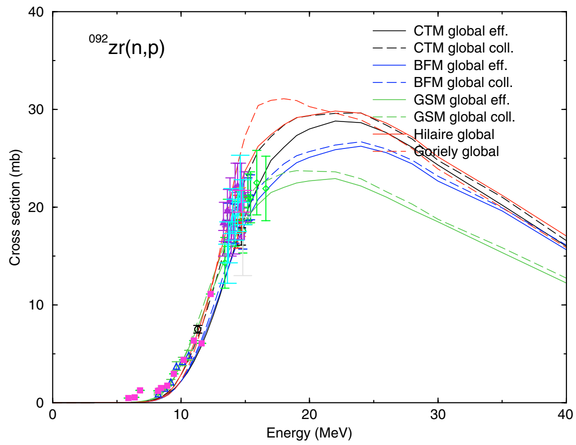

Fig. 2. Blind TALYS calculations for ^{92}Zr(n, p) for various level density models, compared with experimental data.

(n, γ), (n, 2n), (n, p), (n, d) and (n, α) experimental data that were available to us for the entire periodic table of elements. Figure 2 shows ^{92}Zr(n, p) as an example. For all models, including the level densities, global parameterizations were taken. Visual inspection of all target/reaction combinations reveal to what extent the code is stable and has predictive power, and whether our level density models are of decent quality.

4 SALTY: a huge nuclear reaction data library

After verifying that the code produces decent "out of the box" answers, a logical step is to make use of the currently available computer power and put TALYS into mass production mode. The result is SALTY, a nuclear data library produced at NRG which is based entirely on TALYS. The library contains:

- Nuclear data tables for incident neutrons, photons, protons, deuterons and alpha particles.
- Cross sections for all open channels, all secondary angular distributions, double-differential spectra, residual production cross sections, isomeric branching ratios and continuum and discrete photon production, for energies between 10^{-5} eV and 200 MeV and all stable nuclides between F and Bi, both in human-readable x-y tables and as full ENDF-6 transport data files and ACE libraries.
- Cross sections for all open channels, for energies between 10^{-5} eV and 60 MeV for about 1200 nuclides (lifetime beyond 1000 sec.), both in human-readable x-y tables and as ENDF-6/EAF activation data files [21].

Hence, for purely nuclear physics purposes, easy retrieval from the x-y tables gives the default TALYS prediction. For applications, successful NJOY-processing of the ENDF-6 files guarantees the use of these libraries in, at least, MCNPX.

Positive aspects:

- The mutual quality of these isotopic tables is relatively consistent. The same set of nuclear models is used and, equally important for applications, the same ENDF-6 formatting procedures for each isotope. The resulting data files are more complete, in terms of reaction description, that many of the existing individual evaluations.
- "First completeness, then quality".

Negative aspects:

- It is clear that the database needs to be accompanied by a large warning sign: Automatic production means that the data in this evaluation have not been tested against individual experimental data for each isotope, but is only as good as the global quality of TALYS-1.0. Only investing more effort into a single isotope produces truly *evaluated* data files.
- As usual, we run the danger that others compare our blind TALYS results unfavorably to other codes with specific input parameters adjusted to experiment. A similar concern holds for our ENDF-6 files.

Possible future extensions are addition of triton and helium-3 results, more nuclides and energies, and the addition of covariance data to the results. We hope for worldwide validation (with e.g., MCNPX) and feedback.

5 Conclusions

After 8 years of development and two beta versions, TALYS-1.0 is released. We recommend to use the code for any nuclear reaction simulation in the 1 keV–200 MeV energy range. The performance of the code has been established through various individual and global validation cases, and we hope that the results will not be disappointing.

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