EPJ Web of Conferences **284**, 14007 (2023) https://doi.org/10.1051/epjconf/202328414007
ND2022

Current status of the verification and processing system GALILÉE-1 for Evaluated Data

Mireille Coste-Delclaux[1], *Cédric* Jouanne[1,*], and *Claude* Mounier[1]

[1]DES, Service d' Études des Réacteurs et de Mathématiques Appliquées (SERMA), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France

Abstract. This paper describes the current status of GALILÉE-1 [1], the new verification and processing system for evaluated data, developed at CEA. It consists of various components respectively dedicated to read/write the evaluated data independently of the format, to diagnose inconsistencies in the evaluated data and to provide continuous-energy and multigroup data as well as probability tables for particle transport and depletion codes. All these components are written in C++ language and share the same objects. In this paper, we detail the main advances made in GALILÉE-1 : Unresolved Resonance Range (URR) treatment, Thermal Scattering Law (TSL) processing and anisotropy calculations from resonance parameters.

1 Introduction

The GALILÉE-1 system, written in C++ language, is a new verification and processing system for evaluated data. It is part of a CEA global development program dedicated to the modelling of nuclear systems. At the present time, three main components are under development:

- GALION (GALILÉE-1 Input Output for Nuclear data): dedicated to read evaluated data and write produced data.
- GALVANE (GALILÉE-1 Verification of the Accuracy of Nuclear Evaluations): dedicated to verify nuclear evaluations that are GALILÉE-1 input data.
- GTREND (GALILÉE-1 TReatment of Evaluated Nuclear Data): dedicated to provide continuous-energy (CE) and multigroup (MG) data as well as probability tables (PT).

A user-friendly and automatic chain for creating Continuous energy (CE) libraries for the Monte Carlo codeTRIPOLI-4® [2] is under development. Additional components such as interface modules for creating multigroup (MG) libraries for deterministic transport codes will be added later.

2 GALILÉE-1 system description

The GALILÉE-1 system is built upon the GBASE component that defines and implements a set of common objects, shared by all other GALILÉE-1 components. GBASE objects are completely independent from the input and output data formats.

As shown in Figure 1, GBASE objects are initialized thanks to GALION that reads the evaluation or the structure data. These objects are checked and possibly corrected by GALVANE and then processed data are created by GTREND. One has to note that GALVANE and GTREND only work on GBASE objects, which allows the same verification and processing stages, independently of the evaluation format. The objects storing processed data are kept in GBASE and can be written on binary or ASCII files by GALION.

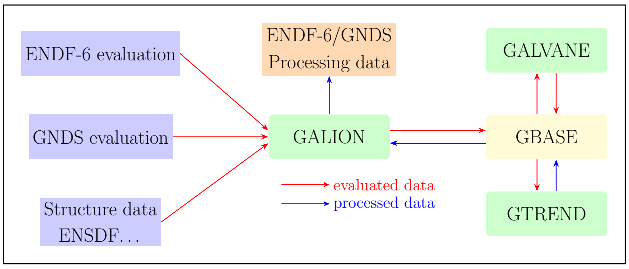

Figure 1. GALILÉE-1 processing modules

3 GBASE Objects

The GBASE object hierarchy is very close to the GNDS [3] object hierarchy. For each nucleus or element, we create a database allowing us to store, in the same object, structure data and interaction data for a given projectile. GBASE structure data contain all the information needed to verify and optionally correct the evaluated data: masses, level scheme, spins, energy, half-life, decay modes, etc. GBASE interaction data contain:

- the list of products that can be created by the interaction,

[*]e-mail: cedric.jouanne@cea.fr

- all the information given in an evaluation (JEFF-3.3 [4], ENDF/B-VIII [5], JENDL-4.0 [6],. . .) but organized in such a way that processing is easier,
- data processed using GALILÉE-1 (CE data, Probability Tables, MG data, . . .).

Several GBASE structure data or several GBASE interaction data may exist in the same database.

4 GALION module

GALION can read evaluated data in ENDF-6 [7] or GNDS (under progress) format as well as structure data in ENSDF or NUBASE format. It supplies tools for creating the GBASE objects corresponding to structure data or interaction data. It also provides tools for writing CE data in PENDF format.

5 GALVANE module

One of the goals of GALILÉE-1 system is to test the consistency and the validity of nuclear data evaluations. We plan to perform a complete assessment of evaluated files before any treatment. Currently, GALVANE can diagnose inconsistencies in general information, resonance parameters, reaction Q values, thresholds, excited level schemes, kinematic data of emitted particles and thermal scattering laws. Some checks can be performed by comparing data with the ones contained in structure databases, e.g. NUBASE or ENSDF. This is the case for:

- masses of nuclides, given in terms of neutron mass,
- energies of excited states reached in the inelastic scattering,
- gamma decay schemes of the excited states.

Some additional tests are designed to check the consistency between the data given in an evaluation:

- consistency between thresholds considered for various data of the same reaction,
- energy balance for reaction products,
- spin/parity of resonance parameters,
- normalization of distributions.

6 GTREND Module

GTREND module aims at replacing NJOY [8] and CALENDF [9] codes in CEA application library production. It consists of three main parts, GTREND_CE corresponding to NJOY/RECONR, /BROADR, /UNRESR, /THERMR and /HEATR, GTREND_PT corresponding to CALENDF, and GTREND_MG corresponding to NJOY/GROUPR. Today, GTREND can reconstruct CE cross-sections in the resolved resonance range, averaged cross-sections in the unresolved resonance range, generate a linearization grid, broaden linearized cross-sections, calculate MG probability tables over the whole energy range (resolved/unresolved/continuum) and CE probability tables in the unresolved range.

7 Probability Table calculation in the Unresolved Resonance Range (URR)

7.1 Calculation method

In this section, we provide some details about probability table calculations in URR. In order to build these data, we need to generate random resonances by sampling physical quantities according to distribution laws given in the evaluation. GTREND has two ways of producing probability tables in URR. The first one (Standard PTs) is similar to the one used by CALENDF. URR is treated in the same manner as the resolved resonance range (RRR); Several random PENDF files are generated on the whole URR, here "random" means that, for each PENDF file, random resonances are generated. That allows using the SLBW formalism to calculate linearized cross-sections to create the random PENDF files. For each random PENDF file, cross section moments are calculated by integration methods developed in GALILÉE-1. These moments are then averaged leading to a moment-based probability table. Usually about 30 random PENDF files are used. The second way (Monte Carlo PTs) can be used to produce either MG or CE PT in URR. As for the first way, random resonances are generated on the whole URR. They are used to calculate cross-sections at various energies (either several energies in a group for MG PTs or given energies for CE PTs). It is important to notice that no linearization step (very time-consuming) is used. The sequence (placing the resonances and calculating the cross-sections) is then repeated a large number of times in order to obtain a cross-section distribution (in each group or at each energy) that is used to calculate the moments by discrete integration. Finally, a moment-based PT can be calculated. Usually, more than 50,000 cross-section samples are used for a group or for a given energy.

7.2 BigTen calculation

We present in this section the results obtained for calculations performed with various PTs for U238 on the ICSBEP/IMF-007-2Z configuration [10]. It consists of a sphere composed of uranium isotopes U234, U235, U236 and U238 surrounded by a shell composed of the same nuclei. For this benchmark, the ENDF/B-VIII.0 library is used. Calculations are performed with Monte Carlo codes MCNP-6.1 (MCNP) [11] and TRIPOLI-4.11.1 with or without probability tables. The PTs used by TRIPOLI-4 are provided either by CALENDF or by GALILÉE-1 with the standard method (Std) or with the Monte-Carlo method (MC). All CE cross sections (PENDF Files) are calculated using NJOY Version 2016 (NJ16).
Table 1 shows the results of the multiplication factors obtained with TRIPOLI-4 and MCNP. All nuclear data are identical for all TRIPOLI-4 calculations, except for the U238 PTs. We can thus estimate the impact of the U238 PTs by comparing the calculations with and without PTs, that is of about 360 pcm. The three results obtained with TRIPOLI-4 and the three sets of probability tables (CALENDF, GTREND-Std and GTREND-MC) are

in good agreement. We observe a significant difference with the MCNP calculation of about 60 pcm. GALILÉE-1 has the capability to compute probability tables for all or some reactions. The PURR module of NJOY generates PTs only for the total, elastic scattering, radiative capture and fission cross sections. If we calculate PTs only with these four reactions, we obtain a multiplication factor in very good agreement with one of MCNP. Figure 2 shows the relative deviations of the neutron fluxes in the unresolved resonance range of U238 (20 keV to 149 keV) from the flux calculated by MCNP. We can thus observe the impact of taking into account the resonance fluctuation of the inelastic scattering cross section on the flux.

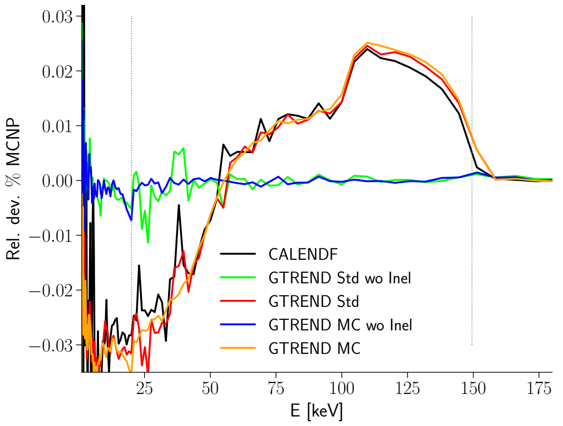

Figure 2. Analysis of neutron flux in IMF-007-2Z. Relative deviation respect to the MCNP flux

These results show that GALILÉE-1 has the capability to produce consistent libraries for TRIPOLI-4 whatever the options chosen (Std or MC) for the calculation of the PTs are.

Table 1. k_{eff} calculated for the BigTen-2Z benchmark using TRIPOLI-4 (T44) and MCNP.

MC Calculations + PT characteristics	Results
T4 without PT	0.99150 (3)
T4 + CALENDF PT	0.99524 (3)
T4 + GTREND PT Std	0.99508 (3)
T4 + GTREND PT MC	0.99509 (3)
MCNP + NJ16 PT	0.99455 (3)
T4 + GTREND PT Std wo inel	0.99450 (3)
T4 + GTREND PT MC wo inel	0.99455 (3)

8 Thermal Scattering Law (TSL) processing

The GTREND module of GALILÉE-1 allows the calculation of thermal scattering laws (TSL) for bound nuclei. We have implemented a calculation mode similar to that of the NJOY/THERMR module that uses a fixed incident energy grid with 117 energies for the calculation of reaction cross sections and for the double differential energy and angle scattering data. We have named this calculation mode GTREND-No-Optimized (GT No Opt.). GTREND has also the capability to optimize the prior incident energy grid given by the user. This prior grid can be halved recursively under a convergence test applied to the total incoherent inelastic scattering. This calculation mode is called GTREND-Optimized (GT Opt.).
The case of H1 in ZrH incoherent inelastic scattering allows us to visualize the impact of this optimized version on the cross section. Figure 3 shows these differences over the energy range between 0.4 and 1 eV. These fluctuations obviously have an impact on the slowing down in a ZrH medium. We can also observe differences on the calculations of the multiplicative factor for the TRIGA configuration (ICSBEP benchmarks ICT-003-1 and ICT-003-2). Table 2 presents the results obtained with TRIPOLI-4 and the JEFF-3.3 library for these two benchmarks. For each configuration, we present three calculations for three different thermal data treatments : NJ16/THERMR, GTREND-No-Optimized and GTREND-Optimized. We observe a very slight impact of the optimized treatment for these configurations.

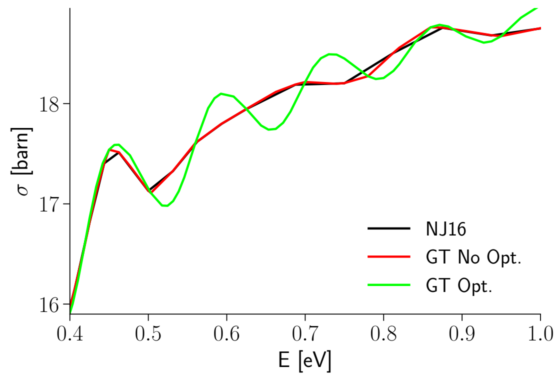

Figure 3. Comparison of incoherent inelastic cross-sections processed for H1 in ZrH

Table 2. k_{eff} calculated for thermal ICSBEP benchmarks (configurations with H1 in ZrH) using TRIPOLI-4

Bench.	NJ16/THERMR	GT No Opt.	GT Opt.
ICT_003_1	1.00740 (4)	1.00742 (4)	1.00776 (4)
ICT_003_2	1.01162 (4)	1.01167 (4)	1.01198 (4)

9 Angular distributions

The angular distributions of neutrons emitted by neutron-induced reactions (elastic and inelastic scattering, . . .) can be calculated using the resonance parameters in the case of the R-matrix Limited formalism. This is also the case for neutron-nucleus elastic scattering with the Reich-Moore formalism. The angular distributions in the center of mass are then expressed using Legendre polynomials following Blatt and Biedenharn [12].

In the case of Fe56 from the JEFF-4.0T1 library, the R-Matrix Limited formalism is used for resonance parameters. Two possibilities are then available for the

anisotropy data of the elastic and inelastic scattering towards the first excited state in the resonance domain (up to 2 MeV): use the anisotropies available in the evaluation file or calculate these anisotropies from the resonance parameters. The RECONR module of NJOY allows to calculate these anisotropies at 0 K for elastic and inelastic scattering when R-Matrix Limited formalism is used, while GTREND allows this type of calculations when R-Matrix Limited or Reich-Moore is used. We processed this evaluation with NJOY and GALILÉE-1 and performed criticality and shielding calculations to investigate the impact of these angular distributions. Table 3 shows results for two criticality benchmarks with a significant influence of Fe56. The difference between the angular distributions from the evaluation (Eval.) and those calculated from the resonance parameters (NJ16 or GALILÉE-1) is about 600 to 700 pcm for these configurations.
We can also observe a significant impact of these angular distributions for the ASPIS shielding benchmark [13] which concerns the propagation of fission neutrons in an iron bulk. Figure 4 shows the C/E ratio for an Rh103 (n,n') dosimeter (40 keV threshold) for the three sets of angular distributions (as in the critical benchmarks). The impact of these anisotropies is very important as the neutrons penetrate into the iron bulk.
It is therefore important that the anisotropies are accurately defined in the evaluation files.

Table 3. TRIPOLI-4 k_{eff} calculated using various angular distribution in resolved range

Bench.	HMF-014	PMF-028
Eval.	1.00048 (10)	1.00569 (10)
NJ16	0.99453 (10)	0.99893 (10)
GALILÉE-1	0.99450 (10)	0.99875 (10)

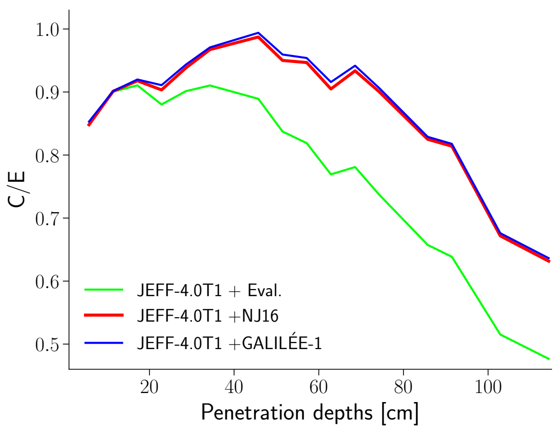

Figure 4. TRIPOLI-4 C/E Rh103(n,n') dosimeter results using various angular distributions in ASPIS benchmark.

10 Conclusions

Thanks to the latest developments of GALILÉE-1 we have now the capability to produce a complete CE library for the Monte Carlo code TRIPOLI-4. The cross-sections reconstruction from resonance parameters and Doppler broadening were already implemented and presented [1]. Important developments have been made for the treatment of the unresolved domain with the new capability of constructing probability tables by two different ways, which already allows us to replace CALENDF for the APOLLO-2 and APOLLO-3® and TRIPOLI-4 codes and to produce in the near future probability tables for MCNP. Thanks to the GALILÉE-1 flexibility, we were able to explain the discrepancies observed between TRIPOLI-4 and MCNP for the Bigten benchmark by the difference in the treatment of the competitive reaction in the unresolved resonance range. The processing of TSL data is also available in GALILÉE-1 and allows reconstructing with an excellent accuracy the incoherent inelastic cross-sections in this energy range. The example of H1 bound in ZrH highlights the importance of this improved reconstruction. The last feature presented here is the reconstruction of anisotropies from resonance parameters for the Reich-Moore and R-Matrix Limited formalisms. We have shown the impact of this treatment for shielding and criticality benchmarks. Future developments planned in GALILÉE-1 will deal with CE libraries and with MG libraries for deterministic codes. One of the objectives is to produce the future libraries for the TRIPOLI-5® code under development at CEA.

References

[1] M. Coste-Delclaux et al., EPJ Web of Conf. **239** 10002 (2020)
[2] E. Brun et al., ANE **82**, 151 (2015)
[3] D. Brown et al., OECD Report **NEA–7519**, (2020)
[4] A. Plompen et al., EPJ A **56**, 1 (2020)
[5] D. Brown et al., NDS **148**, 1 (2018)
[6] K. Shibata et al., JNST **48**, 1 (2011)
[7] A. Trkov et al., BNL **80** (2012)
[8] R. E. MacFarlane et al., LANL, USA,**LA-UR-17_20093** (2017)
[9] J. C. Sublet et al., **CEA-R-6277** (2011)
[10] J. D. Bess et al., EPJ Web of Conf. **239**, 18002 (2020)
[11] T. Goorley, **LA-UR-14-24680** (2014)
[12] J. M. Blatt et al., Rev. Mod. Phys. **24**, 258 (1952)
[13] I. Kodeli et al., Prog. in Nuc. Sc. and Tech. **4**, 308 (2014)