Current status of the verification and processing system GALILÉE-1 for evaluated data

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Abstract. This paper describes the current status of GALILÉE-1 that is 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 whatever the format is, to diagnose inconsistencies in the evaluated data and to provide continuous-energy and multigroup data as well as probability tables for transport and depletion codes. All these components are written in C++ language and share the same objects. Cross-comparisons with other processing systems (NJOY, CALENDF or PREPRO) are systematically carried out at each step in order to fully master possible discrepancies. Some results of such comparisons are provided.

1 Introduction

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 fine modelling of nuclear systems. At the present time, three main components are under development:

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

Additional components, such as interface modules creating consistent libraries for application codes or a convivial and automatic chain for creating these libraries, will be developed later.
GALILÉE-1 system originality lays in its two complementary running ways: an integrated one and an open one for providing application codes with processing tools.

2 GALILÉE-1 system description

GALILÉE-1 system is built upon 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, whatever the evaluation format is. The objects storing processed data are kept in GBASE and can be written on binary or ASCII files by GALION

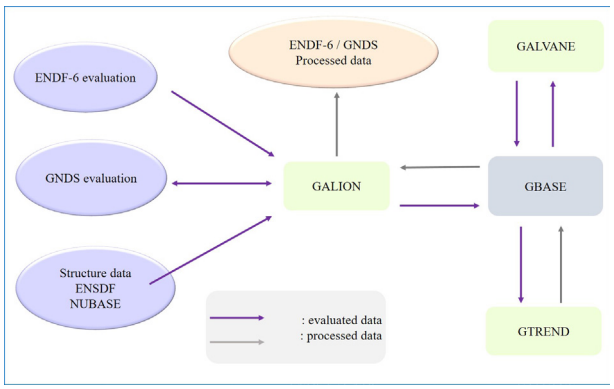

Figure 1. GALILÉE-1 processing modules

3 GBASE Objects

The GBASE object hierarchy is very close to the GNDS 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,

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level scheme, spins, energy, half-life, decay modes, etc. "GBASE interaction data" contain:

- the list of products that can be created by the interaction,
- all the information given in an evaluation (JEFF-3.3, ENDF/B-VIII, JENDL-4.0,...) 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 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 evaluated data. It also provides tools for writing continuous energy data in PENDF format. Currently,GALION is able to read the cross sections in "GNDS 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, Q reaction 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 code aims at replacing NJOY [1] and CALENDF [2] 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 continuous energy cross-sections in the resolved resonance range, averaged cross-sections in the unresolved resonance range, generate a linearization grid, broaden linearized cross-sections, calculate multigroup probability tables over the whole energy range (resolved/unresolved/continuum) and pointwise probability tables in the unresolved range.

6.1 Reconstruction in the resolved resonance range

Formalism

Following references [3] [4] [5] [6], in scattering theory, a channel c is characterized by the pair α of two particles making up the channel, the orbital angular momentum of the pair l, the channel spin s (including associated parity) that is the sum of the spins of the two particles of the pair and the total angular momentum J (including associated parity). A spin group of channels is defined as a set of channels with the same total angular momentum J. The angle-integrated cross-section from entrance channel c to exit channel c', with total angular momentum J , is given, in terms of the scattering matrix $U_{cc'}$, by:

$$\sigma_{c,c'} = \frac{\pi}{k_\alpha^2} g_{J\alpha} |e^{2iw_c}\delta_{cc'} - U_{cc'}|^2 \delta_{JJ'} \tag{1}$$

where k_α is the wave number, $g_{J\alpha}$ the spin statistical factor and w_c is the difference between the Coulomb phase shift for a given l and for $l = 0$ (this difference is equal to zero for non-Coulomb channels). The scattering matrix U, that describes the transition between entrance and exit channels, can be written:

$$U = \Omega[1 + 2iP^{\frac{1}{2}}(1 - RL)^{-1}RP^{\frac{1}{2}}]\Omega \tag{2}$$

- Ω is the diagonal matrix which diagonal term is given by $\Omega_{(c,c)} = e^{i(w_c - \phi_c)}$, ϕ_c being the hardsphere phase shift,
- L is the diagonal matrix which diagonal term is given by $L_{(c,c)} = S_c + iP_c - B_c$, S_c, P_c, B_c being respectively the shift factor, the penetrability and a boundary condition (real functions),
- P is the diagonal matrix which diagonal term is equal to P_c,
- R is the channel matrix which terms are defined by:

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda,c}\gamma_{\lambda,c'}}{E_\lambda - E}\delta_{JJ'} \tag{3}$$

$\gamma_{(\lambda,c)}$ standing for the reduced amplitude, E_λ for the energy of the level, E for the neutron kinetic energy and J and J' for respectively the total angular momentum (with associated parity) of the channel c and c'. The scattering matrix U can be written in terms of X matrix as:

$$U = \Omega[1 + 2iX]\Omega \tag{4}$$

$$X = P^{\frac{1}{2}}(1 - RL)^{-1}RP^{\frac{1}{2}} \tag{5}$$

In GTREND, the angle integrated cross-section for the interaction leading from particle pair α, for which one particle is a neutron, to particle pair α', is deduced from X

matrix in the following way:

$$\sigma_{\alpha\alpha'} = \frac{4\pi}{k_\alpha^2} \sum_J g_{j\alpha} \sum_c [(\sin^2(\phi_c)\,(1 - 2Im(X_{cc})) - \sin(2\phi_c)\,Re(X_{cc}))\delta_{\alpha\alpha'} + \sum_{c'} |X_{cc'}|^2] \quad (6)$$

The summations are over channels c and c' belonging to the spin group J and such that the particle pair is α for c and α' for c'. The nuclear formalisms currently supported in GTREND are Single and Multi-level Breit-Wigner, Reich-Moore, and R-Matrix-Limited formalisms. The classical approximations are implemented.

Results

In order to validate GTREND reconstruction at 0 Kelvin in the resolved resonance range, cross-comparisons with NJOY2016 were carried out for all JEFF-3.2 nuclei (470). About 25 nuclei show relative reconstruction discrepancies larger than 10^{-5}, between NJOY2016 and GTREND, for MT1, MT2, MT102 and MT18 when it exists. All observed discrepancies have been explained. Figure 2 shows a comparison of the total cross-section reconstructions with NJOY2016 and GTREND.

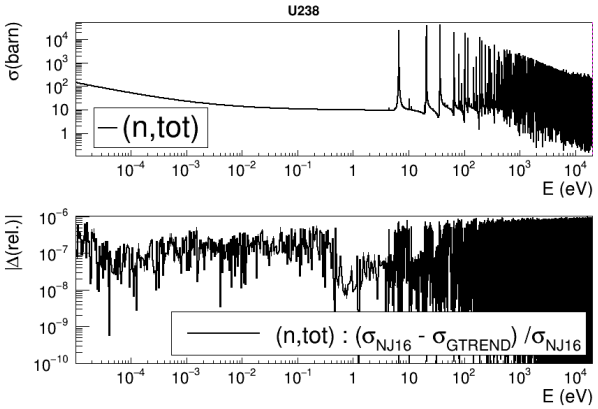

Figure 2. Comparison between NJOY2016 and GTREND on U238 reconstruction in RRR

6.2 Linear piecewise reconstruction

A tool building a piecewise linear approximation of the cross-sections derived from a nuclear formalism (accurate but time consuming) is very convenient and efficient for the processing itself and for Monte Carlo transport codes. In the frame of GALILÉE-1, we developed a generic linearization tool. Various concrete criteria are implemented such as Punctual, Integral or Mixed ones. When an integral criterion is used a weighting function W is mandatory. The function F to be represented in a piecewise linear form has to be a "functor" with a specific signature. This allows us to use the same algorithm for various types of functions: resonance formalism, thermal scattering model, Legendre expansion of an angular distribution or tabulated function with various interpolation schemes. The user must give, as input data, well-chosen points in the linearization range.

The basis of the GALILÉE-1 algorithm is very similar to the one implemented in NJOY: halving interval and checking with some kind of criteria. The first two basic criteria are the maximum number of subdivisions of an initial interval and the minimum width of an interval expressed in term of a multiple of the machine epsilon. All the specialized criteria use these two parameters.
A convergence diagnostic is available to check if the "convergence" is reached using these criteria. The diagnostic can be used to trigger a restart of the linearization process with the same or with modified parameters of the criterion. This restart mode is useful if the user cannot set properly the initial points of the linearization.

6.3 Doppler Broadening

Description

The Doppler broadening and the thermal modules are designed consistently in GTREND whatever the thermal motion is (free gas or chemical binding model). The Doppler broadening and the calculation of thermal scattering cross-sections can be done starting from a nuclear cross-section given by the true formalism or from a linearized one. Right now, only the "SIGMA1" method designed in PREPRO [6] system that provides an exact Doppler broadening for a piecewise linear representation of a cross-section, is implemented in GTREND. This algorithm is certainly one of those that give the best results in terms of accuracy even if it is not the fastest. We will also benefit from the PhD work done at CEA on multipole processing [7].

Results

For validating GTREND, we performed, on U238 JEFF-3.2, a SIGMA1 Doppler broadening at 300K on the NJOY2016/BROADR energy grid and we compared the cross-sections to the NJOY ones. The relative discrepancies are given in Figure 3. The comparison is satisfactory (upper plot) but at high energies, NJOY2016 processing may generate unphysical behaviors for radiative capture cross section (lower plots). The emergence of these peaks below the energetic position of a resonance induced by the Doppler broadening using NJOY has already been observed when NJOY is compared with PREPRO or with GRUCON (Russian code)[8]. We have an excellent agreement with PREPRO in this case. We have chosen in this article to present a comparison with NJOY which is the most used code.

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

In this section, we present the first results on probability table calculations in URR. In order to build these data, we need to sample physical quantities according to distribution laws given in the evaluation: spacing between the resonances is distributed according to the Wigner's law and partial widths are represented by χ^2's laws with various degrees of freedom.
GTREND has the capability to produce probability tables for two types of representation and use:

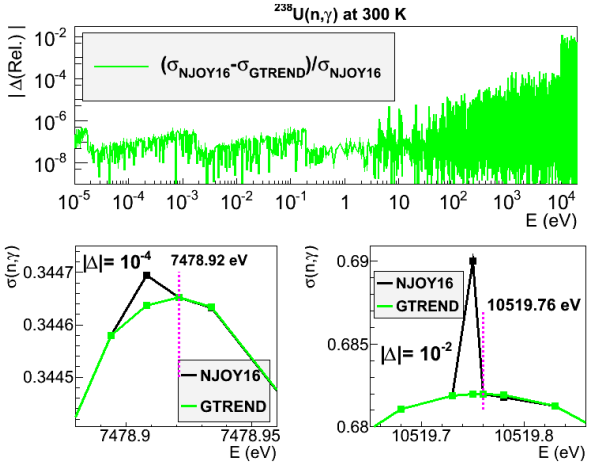

Figure 3. Relative discrepancies on radiative capture cross-sections of U238 at 300 K

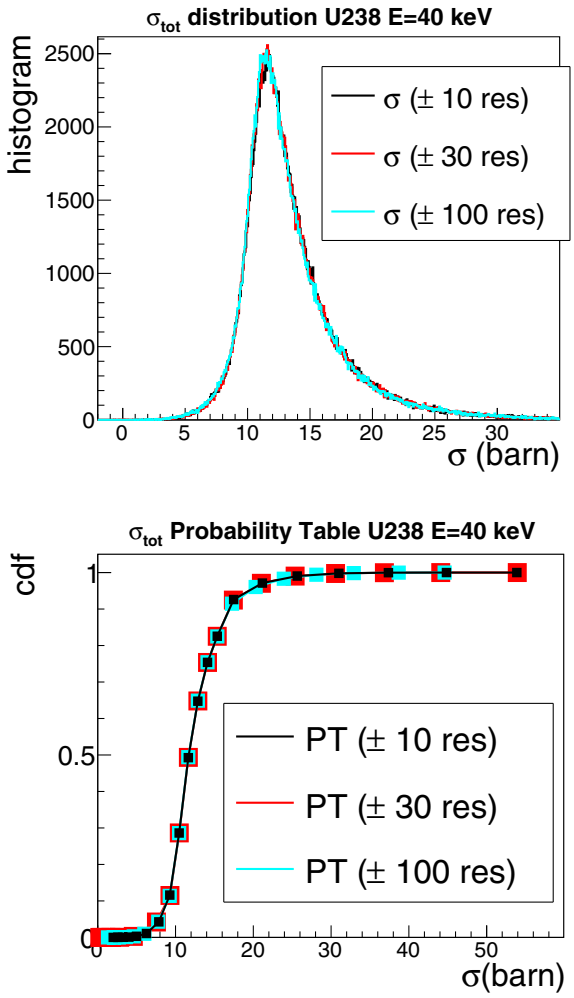

Figure 4. Probability table construction, U238 at 40 keV

- NJOY/PURR-like probability tables for use with the Monte Carlo code MCNP for example. These tables are calculated on a few number of energy points in the URR domain.
- CALENDF-like probability tables for use with the Monte Carlo code TRIPOLI-4® or the deterministic codes APOLLO-2 and APOLLO-3®. These tables are given on a multigroup energy mesh over the whole energy domain.

NJOY/PURR-like probability tables

We have undertaken various tests to validate the calculation of these probability tables. In a first time, we sampled 500,000 sets of random resonances to define the distribution of the cross sections on a given energy grid in the unresolved domain. The nucleus selected was U238 from JEFF-3.2 library that contains URR from 20 keV to 149 keV. We were concerned with the influence of the number of resonances taken into account around the energetic position for the calculations. We sequentially considered 20, 60 and 200 resonances around this computational energy. Figure 4 shows the histograms of the 500,000 total cross section values calculated at 40 keV for this nucleus as a function of the number of resonances taken into account (upper plot). In agreement with the common representations for MCNP, we calculated the 20-step probability tables from the total cross sections for these three histograms. The lower plot of Figure 4 shows the cumulative distribution of these probability tables. We observe a very good agreement, whatever the number of resonances taken into account is, for the calculation of the cross sections in this case. We have to generalize this test for different nuclei in order to define a processing methodology for the reconstruction of probability tables.

CALENDF-like probability tables

GTREND has the capability to produce multigroup moment-based probability tables following the method used in CALENDF. In the resolved or continuum energy ranges, moments to be preserved are calculated using the exact or the linearized cross section.

In the unresolved resonance range, we distribute resonances over a domain that covers the whole unresolved domaine but also the high part of the resolved domain and the low part of the continuum, by applying the distributions defined in the evaluation files. That allows us to obtain a correct representation for groups close to the boundaries of the unresolved domain. Using this series of resonances, we reconstruct a pointwise pseudo cross section in the unresolved domain. The upper plot of Figure 5 presents the U238 total cross section over the whole energy range. In the URR range, the black curve is the average cross section while the red curve is an example of a random pseudo cross section. The black curve contains 160,000 energies from $10^{-5}\,eV$ to $20\,MeV$, the red curve requires 470,000 additional energies over the unresolved range. The lower plot of Figure 5 shows three pseudo cross sections in the unresolved domain and the average cross section calculated from the average parameters given in the evaluation. The probability tables used in the following section for uranium 238 are calculated from thirty series of random

resonances and then from thirty pseudo cross sections in the unresolved domain.

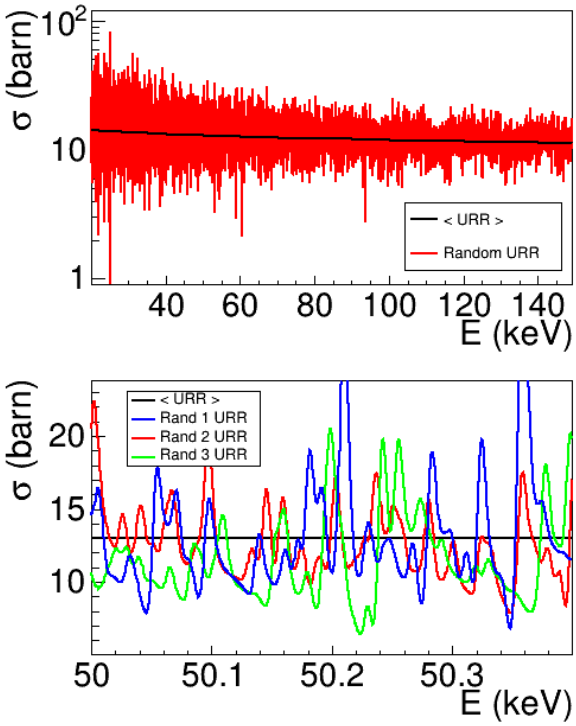

Figure 5. U238 : random pseudo cross sections in URR

7 BigTen calculation

We present in this section the results obtained for various calculations performed on the ICSBEP/IMF-007-2Z configuration. It consists of a sphere composed of uranium isotope U234, U235, U236 and U238 surrounded by a shell composed of these same nuclei. For this benchmark, the JEFF-3.2 library is used. Calculations are performed with Monte Carlo codes MCNP-5.1.40 and TRIPOLI-4.11 with or without probability tables. The calculations performed are :

- T4+NJ16 + CALENDF: pointwise cross sections and probability tables are respectively produced using NJOY2016 and CALENDF. Calculations are performed with TRIPOLI-4
- T4 + GTREND: pointwise cross sections and probability tables are produced using GTREND. Calculations are performed with TRIPOLI-4
- MCNP + NJ16: Calculations are performed with MCNP and libraries are produced using NJOY
- MCNP + GTREND: Calculations are performed with MCNP. Pointwise cross sections and probability tables are produced by GTREND
- T4 + 30 random PENDF: pointwise cross sections on the whole energy domain (including URR) are calculated using GTREND. The pointwise cross sections used in URR are described in the previous paragraph. Calculations are performed with TRIPOLI-4.

Table 1 presents the different k_{eff} calculated for this BigTen two zoned homogenized benchmark. The four calculations performed without probability tables using MCNP and TRIPOLI-4 are in very good agreement which shows a good accuracy for GTREND pointwise cross sections.
The use of probability tables in the Monte Carlo codes MCNP and TRIPOLI-4 increases the calculated k_{eff} by about 400 pcm. The T4+GTREND, MCNP+NJ16 and MCNP+GTREND calculations are in very good agreement. The T4+NJ16+CALENDF calculation gives a slightly higher k_{eff} by 60 pcm. The experimental value expected for this configuration is 0.99480±300pcm. It doesn't discard any of these calculations.
The last result of Table 1 is the average of the k_{eff} calculated with the thirty pseudo PENDF files. The average k_{eff} obtained is in very good agreement with the calculations performed using probability tables and with the expected experimental value.

This results show that GTREND has the capability to produce consistent libraries for MCNP and TRIPOLI-4 which was not possible until now.

Table 1. k_{eff} calculated for the BigTen-2Z benchmark

MC Calc + XS Prod.	without PT	with PT
T4 + NJ16 + CALENDF	0.99040 (5)	0.99506 (6)
T4 + GTREND	0.99045 (5)	0.99444 (13)
MCNP + NJ16	0.99043 (5)	0.99440 (6)
MCNP + GTREND	0.99045 (5)	0.99421 (5)
T4+ 30 rand PENDF	0.99465	

8 Conclusions

GALILÉE-1 currently allows the production of consistent libraries for pointwise Monte Carlo transport codes (MCNP and TRIPOLI-4). The cross sections are reconstructed over the whole energy range and Doppler broadened over the energy domain given by the user. Pseudo cross sections are generated to build probability tables in the unresolved resonance range.
As far as cross sections are concerned, cross comparisons have been made with NJOY and PREPRO. In a general way, a very good agreement has been obtained and all residual differences have been explained. For probability tables, as direct comparaisons are not easy, criticality calculations are used for a posteriori validation.
In order to perform MCNP calculations, GTREND was used for generating pointwise probability tables and linearized cross sections. The ACER/NJOY module was then used for creating complete formatted "acefiles". The first calculations performed with MCNP and TRIPOLI-4 on criticality configurations were in very good agreement.

In a near future, GALILÉE-1 will be able to read the evaluation files in GNDS format. Thermal scattering data processing will also be carried out in order to prepare com-

plete libraries for TRIPOLI-4. The production of multi-group libraries for deterministic codes will follow.

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