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 the 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 and write input and 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.

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.

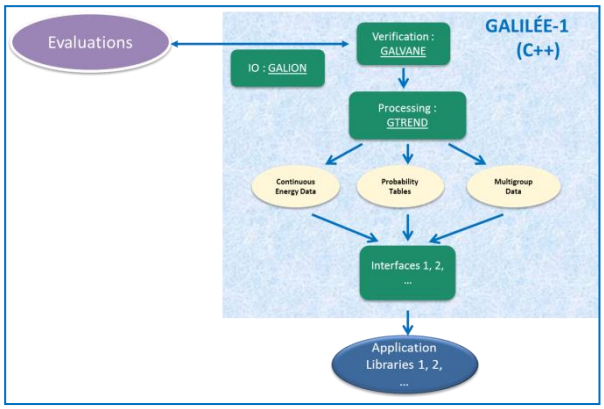


Fig.1 GALILÉE-1 integrated running way.

GALILÉE-1 system originality lays in its two complementary running ways: an integrated one (Fig. 1) and an open one for providing application codes with processing tools (Doppler on the fly for instance).

2 GALILÉE-1 system description

GALILÉE-1 system is built around 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.

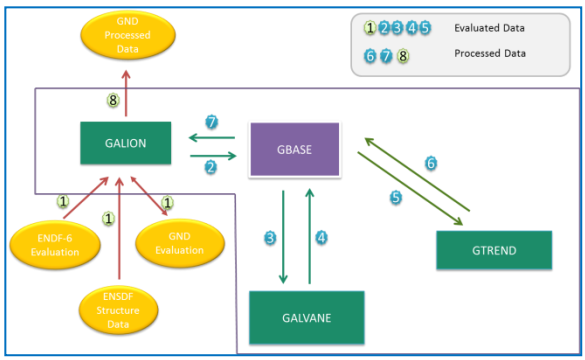


Fig. 2. GALILEÉ-1 processing modules.

As shown in Fig. 2, GBASE objects are initialized thanks to GALION that reads the evaluation or the structure data. These objects are checked and eventually 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

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processed data are also kept in GBASE and can be written on binary or character files by GALION.

3 GBASE Objects

The GBASE object hierarchy is very close to the GND object hierarchy. For each nucleus or element, we create a data base 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, all the information given by an evaluation (JEFF-3.2, ENDF/B-VII.1, JENDL4.0,…) but organized in such a way that processing is easier, and also processed data (CE data, Probability Tables, MG data, …). Several GBASE structure data or several GBASE interaction data may exist in the same data base.

4 GALION

GALION can read evaluated data in ENDF-6 or GND (under progress) format as well as structure data in ENSDF or NUBASE format. It creates the GBASE objects corresponding to structure data or interaction data. Other GBASE objects are under construction. Writing is not yet available but in the future, GALION will also have the capability of correcting an evaluation in GND format.

5 GALVANE

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, 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 coherence between the data given in an evaluation:

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

We present below a list of tests already considered in our code system allowing us to diagnose a list of inconsistent values in an evaluation.

5.1 Target Mass and Q-value reaction

The target mass is very important to determine the Q-value and the threshold of a reaction. In JEFF-3.2 library, the H2 evaluated mass, in neutron mass, is 1.995712 instead of 1.9968 (underestimation of 1 MeV). This discrepancy should impact radiative capture Q-value but it is not the case, the correct Q-value being given in the evaluation. Other examples of important discrepancies can be found in JEFF-3.2 evaluations: for example, more than 4.5 MeV for Xe134 and 366 keV for Ti46. In the case of transfer reactions, one can observe Q-value discrepancies higher than 1 MeV. Moreover, those values are not systematically given.

5.2 Resonance state spin (J value)

The spin of a resonance state, J , is calculated from the orbital angular momentum ℓ, the neutron spin and the target spin I. For Bk247 which spin is 3/2, in agreement with Nubase, the J value given in JEFF-3.2 for s resonances ($\ell = 0$), is *3/2*, out of the range of possible values, 1 or 2. This discrepancy has a significant impact on the calculated cross-section due to the spin statistical multiplicative factor.

5.3 Energy balance for emitted particles

Evaluations contain energetic distributions for emitted particles at various incident energies. From these distributions, we can reconstruct total and partial average energies and compare them to available energy for the reaction. Interpolation schemes for emitted energy distributions and for incident energies play an important role to determine energy release. By analyzing these distributions, we are able to highlight inconsistencies.

5.4 Negative angular distribution

Angular distribution of emitted particles can be represented by Legendre polynomial expansion coefficients. This representation is particularly efficient in terms of compactness. However, the truncation at a given order can produce negative values for angular probabilities.

5.5 Comparisons between libraries

Table 1 shows a comparison of various major data for three distinct libraries: JENDL-4.0, ENDF/B-VII.1, and JEFF-3.2. The number of target files and the number of target files that contain radioactive production are indicated below the name of each library.

Table 1. Comparison of various major data

	JENDL-4.0 (406 / 3)	ENDF/B-VII.1 (423 / 41)	JEFF-3.2 (472 / 169)
Mass comparison	4	27	24
Resonance parameters	0	3	9
Q-reactions	5	92	53
Anisotropy	5	39	35
Decay data	1	14	41
Missing gamma production	139	138	104

Here are some explanations on Table 1 items:

- Mass comparison: Target masses comparison between evaluation file and NUBASE data.
- Resonance parameters: Inconsistencies on the spin of the resonances (J value).
- Q reaction: Inconsistencies on Q-values displayed on evaluation, possibly connected to a target mass default.

- Anisotropy: Negative angular distributions related to Legendre polynomial truncations or wrong normalization of a $(\mu, p(\mu))$ distribution.
- Decay data: Inconsistency on the identification of radioactive products between data in General Purpose evaluation file and ENSDF file or Decay Data evaluation file.
- Missing gamma production: No gamma production for radioactive capture (MF6, MF12 and MF13).

The value in each cell shows the number of affected files, not the total number of reactions.

6 GTREND

GTREND code aims at replacing NJOY99 [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 treatment and GTREND_MG corresponding to NJOY/GROUPR.

Today, GTREND can reconstruct continuous energy cross-sections in the resolved resonance range, provide a linearization grid, broaden linearized cross-sections and calculate moment based probability tables.

6.1 Reconstruction in the resolved range

6.1.1 Formalism

Following references [3] and [4], 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 momemtum J , is given, in terms of the scattering matrix $U_{cc'}$, by:

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

where k_α is the wave number, $g_{J\alpha}$ the spin statistical factor and w_c the Coulomb phase shift difference (equal to zero for non-Coulomb channels).

The scattering matrix U, that describes the transition between entrance and exit channels, can be written:

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

- Ω is the diagonal matrix which diagonal term is given by $\Omega_{c,c} = e^{-i(w_c - \varphi_c)}$, φ_c being the potential-scattering 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:

$$\mathrm{R}_{c,c'} = \sum_\lambda \frac{\gamma_{\lambda,c}\gamma_{\lambda,c'}}{E_\lambda - E}\delta_{JJ'} \qquad (3)$$

$\gamma_{\lambda,c}$ standing for the channel 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:

$$U = \Omega[1 + 2iX]\Omega \qquad (4)$$

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

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:

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

The summation 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 formalisms, Reich-Moore formalism and R-Matrix limited formalism when no Coulomb channel exists. The classical approximations are implemented.

Results

In order to validate GTREND reconstruction at 0 Kelvin in the resolved resonance range, cross-comparisons with NJOY99 were carried out for all JEFF-3.2 nuclei (~ 470). In case of discrepancies, additional comparisons were made with NJOY2012 and PREPRO2015 [5]. About 25 nuclei show relative reconstruction discrepancies larger than 1.E-5, between NJOY99 and GTREND, for MT1, MT2, MT102 and MT18 when it exists.

On MT2 reconstruction, we observe relative discrepancies for Fe54 (≤ 1.26 E-3) and Os192 (≤ 2.01 E-4), not yet fully understood.

On MT102 reconstruction, discrepancies occur for C13, Kr86, O17, O18, Pb206, Pb208, Sr88 and Sr90. This problem disappears with NJOY2012 (except for O17 and O18) and with PREPRO2015 for O18.

On other nuclei, discrepancies may appear on MT1 reconstruction, either when summing the background cross-sections or because of threshold problems. For the reconstruction, GTREND uses the partial cross-sections and not the redundant cross-sections. Moreover, as NJOY does, GTREND modifies the threshold given in the evaluation when its value is not correct. But some differences remain. As an example, for O16 in JEFF-3.2, the MT107 background file is not consistent with the sum of the MT800-MT803 files, above the threshold of the first excited state of C13 (MT801). This problem is solved with NJOY2012.

Moreover, in order to validate R-Matrix limited formalism implementation, new Cielo Fe56 (Dist. April

2014 – ORNL4/ L. Leal) was reconstructed and results were compared with NJOY2012 ones (Fig. 3). For all resonant partial cross-sections, GTREND and NJOY2012 are in excellent agreement. The relative discrepancies are always less than 10^{-5}, except, for the inelastic cross-section, at the two first energies after the threshold where they reach 2.3 10^{-5}.

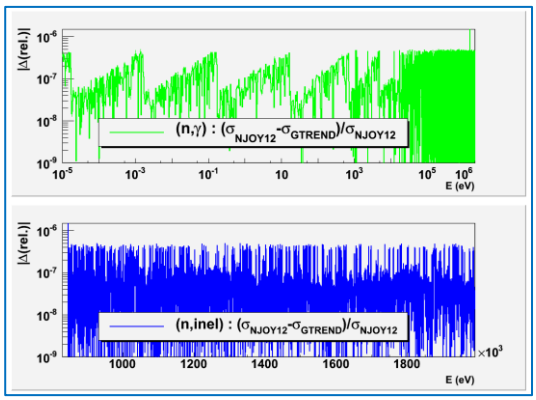


Fig. 3. Relative discrepancies on Fe56 reconstruction

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. 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 reconstruction 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 modified parameters of the criterion. This restart mode is useful if the user cannot set properly the initial points of the reconstruction.

6.3 Doppler Broadening and thermal modules

Description

The Doppler Broadening and the thermal modules will be 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 will be done starting from a nuclear cross section given by the true formalism or from a linearized one. At the present time, only the "SIGMA1" method designed in PREPRO system that provides an exact Doppler Broadening for a piecewise linear representation of a cross section, is implemented in GTREND.

Results

For validating GTREND, we performed, on U238 JEFF3.2, a SIGMA1 Doppler broadening at 294K on the NJOY/BROADR energy grid and we compared the cross-sections to the NJOY ones. The relative discrepancies are given in Fig. 4. The general trend is satisfactory but at high energies, NJOY99 curve may display unphysical behaviors leading to higher discrepancies. Some of them are corrected in NJOY2012.

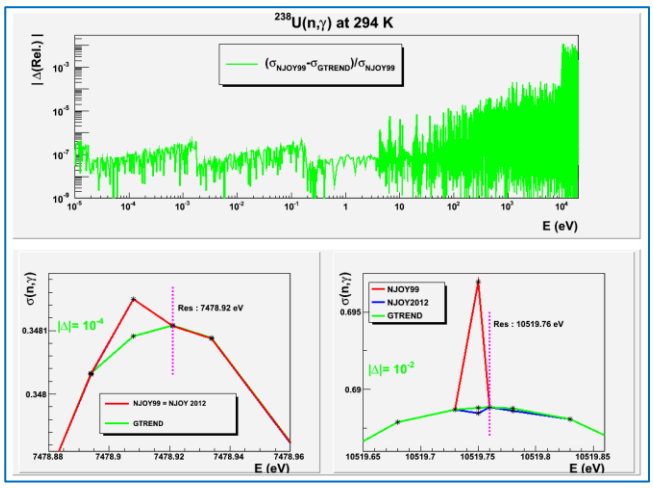


Fig. 4. Relative discrepancies on U238 broadening

7 Conclusion

GALILÉE-1 system will have soon the capability of producing Monte Carlo transport libraries from validated evaluations, which is a first important step for our renewed library creation chain. It allows R&D activity on new processing methods and is also a powerful tool for nuclear data analysis.

References

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