J-GAMUT code: present status

Balraj Singh

Physics and Astronomy, McMaster University, Canada

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Background:

June 2014 IAEA-ENSDF-codes meeting: I proposed a new code to:

1. Automatize deduction of Adopted Gamma-ray energies and photon (γ) branching ratios from multiple datasets for a nuclide. (Most of the work at present is done manually, following a gamma-by-gamma approach.
2. Revive Rick Firestone's GAMUT code in Fortran from the 80's, and rewrite in a modern language such as JAVA. (R. Firestone: LBL-26024 (1991): GAMUT: A Computer Code for γ-ray Energy and Intensity Analysis).

Sept 2014 – Aug 2015: Michael Birch worked on this code with financial support from the IAEA-NDS, and with my input about format and procedures. This code also needed V_AVELIB, rewritten in JAVA from its previous version in Visual-Basic. [Asymmetric uncertainties in JAVA V_AVELIB code were handled differently, following a modified R. Barlow's (arXiv:physics/0406120v1 (2004)) approach].

October 2015 IAEA-ENSDF codes meeting: Michael's presentation of this code, together with a simple example. This version did not create an output file of Adopted Levels, Gammas in .ensdf format.

Corrections and improvements during 2016-2018

The code was released to the network around the end of 2015.
Sometime in 2016, I found that the recoil correction for γ rays had inadvertently been left out (valid for only the GAMUT routine). In 2017 Michael modified the code: to include the correction prior to fitting the γ-ray energies to a level scheme, then remove it in the output file of recommended γ-ray energies.
Also added an option to create an output .ensdf dataset of "Adopted Levels, Gammas" for the two approaches: gamma-by-gamma, and GAMUT. This version was made available in July 2017.

Around 2018, several other bugs came to attention, some through the network evaluators, but mainly when Sorin Pascu (from Bucharest) and I tried this code for the first time on a real-life situation on two nuclei in A=130 evaluation, where a large number of datasets needed to be analyzed: ^{130}Xe and ^{130}Te. Most of These issues were in the GAMUT routine, but some also in Gamma-by-gamma.

Clarification about singular matrix

Singular matrix problem warning: Michael's reply Feb 6, 2018.

"The warning about singular behaviour comes up if the matrix it constructed to represent the level scheme has determinant equal to zero, i.e. the inverse does not exist. However, the code actually uses something called **singular value decomposition** to compute the inverse; a process which produces the usual matrix inverse in cases where the input is invertible, but something called the **Moore-Penrose pseudo-inverse** in cases where the determinant is equal to zero. The pseudo-inverse has many nice properties and in some sense is the best you can do when the proper inverse does not exist, however I thought it would be good to include a warning because there might be some unexpected behaviour in the result (like the negative level energies) and it might be indicative of a problem in the input file. From linear algebra we know that a matrix is not invertible if and only if there is some redundancy in its rows/columns. This redundancy likely arises from somewhere in the ENSDF input, so perhaps you can track it down".

Corrections and improvements…

Bugs: 1. Some Eγ values came out as negative, when only one gamma from a level to the g.s. and listed in the dataset without any uncertainty. For such γ rays, intensities came out with large (wrong) uncertainties. Reason: by default, the uncertainty was set at 30% for non-numeric or missing values. Now one can override this, and set one's own uncertainties e.g. 20% for AP intensity, and 1or 2 keV for energy given as AP. Entries with GE, LE, GT, LT, CA, SY in uncertainty field: ignored. Also other issues with uncertainties. Resolved March 2018.

2. transcription from original datasets to intermediate file was adding extra zero in the numbers for energies and uncertainties in some cases, mainly when a number was stated to the nearest tenth of a keV (i.e. one decimal place): comment from Caroline Nesaraja (ORNL). While not a serious mistake, still needed a correction as decimal place in a number is important in .ensdf format, as it denotes precision. Resolved May 2018.

Corrections and improvements

3. Duplicated entries in the output file for gamma-by-gamma approach: when only one gamma from a level. GAMUT still calculated γ branching ratios when all the gamma rays from a level were unresolved doublets.
Fixed June 2018. However Michael suggested a general warning:
"It should be noted though that the auto-generated ENSDF output has always been unreliable – it is meant to be a template to save some copying and pasting, but needs a thorough review by the evaluator".
4. The doubling problem in the .ens file generated in 'gamma-by-gamma' mostly gone, but still present in one type of entries: for some reason, in the intermediate file, some of the gamma-ray energies get converted to exponential format, mainly when there is only one gamma from a level, for example in (γ,γ ') dataset for ^{130}Xe. Such entries then got doubled in the .ensdf output. GAMUT output seemed fine. Resolved Nov 17, 2018. This version was sent to IAEA-NDS, and was circulated to the network for trial.

Overall experience with ^{130}Xe and ^{130}Te datasets.

Both approaches i.e. gamma-by-gamma and GAMUT were tried:
GAMUT gives Eγ as level-energy differences, a departure from our general approach of recommending Eγ values based only on measured gamma-ray energies. In my opinion, it is still a basic question that has never been answered satisfactorily: what are the best recommended gamma-ray energies from gamma-ray experiments? Similarly what are the best alpha-particle energies in decay schemes involving alpha decays.
So we took Eγ values from gamma-by-gamma approach. With that level energies given by GAMUT were not quite consistent with Eγ from the other method, then we ran the GTOL code to obtain level energies.
Intensities were taken from GAMUT analysis.

Testing of the code

In December 2018, data files for several nuclides downloaded from the ENSDF database were tested by E.A. McCutchan at NNDC. For nuclides with many gamma-ray datasets, the code got stuck in some loop and did not produce intermediate file. In other cases, where the intermediate file was produced, it was found that the level matching was incorrect in cases where level energies were close together, within 5 keV or so. I suggested to Michael to add an option in the code so that a user could annotate closely spaced levels with labels, e.g. letter A and B for two such levels in column 9 in each dataset where these particular levels are populated, then the code reads this label and overrides the general level matching algorithm for such levels. One could continue with such labeling scheme with C, D, etc. for other pairs of levels. During December 2018 to March 2019, Michael improved the code, such that intermediate file gets produced within less than 5 minutes, even for very large data files. In addition the option for annotating closely-spaced doublets or multiplets was added. On April 2, 2019, a modified version of this code was circulated to the network through the IAEA-NDS for further testing.

It should be noted that this code will not work as a black box. Thorough checking of the intermediate file is needed to be able to obtain a meaningful averaged file in the two approaches, and finally an ENSDF-formatted Adopted dataset.

J-GAMUT Demonstration

The working of the March-2019 version of the code was demonstrated using Pt-190 data file, extracted from the A=190 update for ENSDF that has been recently submitted.

The code can be downloaded from the IAEA-NDS webpage. Queries and problems should be addressed to me (balraj@mcmaster.ca).