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Improvement of Analysis Codes for Nuclear Structure and Decay Data Evaluations

Summary of the Technical Meeting

IAEA Headquarters, Vienna, Austria
3-7 December 2018

Prepared by

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February 2019

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ABSTRACT

A summary is given of a Technical Meeting assembled to review the progress in improving and developing new analysis and utility codes used in the evaluation of nuclear structure and decay data for the Evaluated Nuclear Structure Data File (ENSDF). Participants reviewed the existing and newly developed codes and discussed outstanding issues such as the consistent treatment of uncertainties, extending the ENSDF format to accommodate continuous data, updating the ENSDF manual and maintaining user-friendly online webtools and editors. Details of the discussions and the proposed actions are presented in this summary report.

February 2019

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1. Introduction

The ENSDF Analysis and Utility codes are essential tools for the international network of Nuclear Structure and Decay Data (NSDD) evaluators' work and for that reason it is important that they are maintained, i.e. that they are continuously checked for bugs, kept up-to-date with developments in physics models, statistical methods and error analysis, new formats and evaluation methods/policies in general.

The Nuclear Data Section is coordinating an effort to bring together code developers, evaluators and nuclear physics experts to discuss needs for development, improvement and extension of these codes and make recommendations to the code developers and user community.

Two meetings have been held so far, the kick-off Technical Meeting from 10 to 13 June 2014 and a second meeting to monitor progress from 10 to 14 October 2015. The meetings produced a priority list of codes that require either revision or improvement or to be re-written in a modern programming language. They also resulted in recommendations for a uniform and consistent treatment of uncertainties and the consideration of new formats to accommodate new types of data. The summary reports were published in INDC(NDS)-0665 and INDC(NDS)-0696, respectively.

Since then, significant progress has been made leading to the release of new ENSDF analysis and checking codes, including a new publication code. In addition, new proposals have been developed for treating asymmetric uncertainties and for incorporating continuous data in ENSDF meriting further discussions and recommendations. For those purposes, the third meeting of the project was held from 3 to 7 December 2018, at the IAEA.

Eight participants from six countries, including two IAEA staff attended the meeting. A. Sonzogni (BNL) was elected Chair of the meeting while T. Kibedi (ANU) was appointed Rapporteur. The meeting began with presentations given by the participants and continued with technical discussions and recommendations. Summaries of the presetantions are given in Section 2, while the technical discussions are summarized in Section 3. The perspectives are presented in Section 4. The Agenda, list of participants and links to the presentations are provided in Annexes 1-3.

2. Summaries of presentations

2.1. Editors and Web Tools, Viktor Zerkin, IAEA

The main purpose of MyEnsdf is to run ENSDF codes on user's ENSDF file on the Web server. The system allows the user to run remotely the following codes: FMTCHK, chk_ENSDF, PREPRO, XPQCHK, ALPHAD, BrIcc, BrIccMixing, GABS, GTOL, LOGFT, PANDORA, RADLST, RULER, NDSPUB.

Codes and features recently added to MyEnsdf:

- **chk_PARENT**: checking PARENT-records in DECAY datasets/PNPI, ver.24-Jan-2009/
- **chk_brackets**: pair brackets checker for ENSDF-format files/PNPI, ver.20-Apr-2012/
- **ENSDF_to_XML**: converts file ENSDF to XML /PNPI, ver. Nov-2016/

- **ALPHAD_RADD**: alpha hinderance factor program (AHF, AHFYE, ALPHAD) /v-2.0a + RadD:16-Aug-2016/
- **BARON**: calculates model parameters for nuclear rotation bands/PNPI, ver.23-Jun-2014/
- tables with summary of ENSDF file: list of datasets and nuclides allowing to extract dataset/nuclide; list of NSR-references with information from NSR database, links to web-journals and PDF files;
- links to display ENSDF file by viewers and call web editor.

Web viewers and editor:

- **Ensdf+** displays ENSDF file as original "ENSDF cards" and interpretation including ENSDF symbols, NSR KeyNo with link to Web NSR and PDF file (if any), plotting of decay schema (simplified) and gamma transition with indication of possible mistakes, etc.; has interactive functionality limited to hiding/showing selected sections;
- **Ensdf±** presents ENSDF file as an interactive tree-graph, a modern style for displaying the ENSDF file structure. Interpretation is similar to Ensdf+.
- **ENSDF Web-Editor**. Currently it is based on Ensdf± view extending every node by sets of operations (add, remove, edit, etc.). Operations are implemented on pop-up window using the interpretation of ENSDF fields and an automatized input system. Alternative approach for organizing editor's view and operations were discussed.

2.2. Nuclear_refs_manager, Alexander Rodionov, PNPI

The program package Nuclear_refs_manager was described. This is a software manager of references for publications in nuclear physics. The package may be useful for maintaining a collection of publications, i.e. articles, abstracts, private communications, etc., on a PC or laptop, which have keywords following the format of the bibliographic database Nuclear Science References (NSR), Brookhaven National Laboratory. The user can group the collection in journals, years of publication, authors, themes, etc. The search can be customized by journals, year of publication, authors, keywords and keynumbers, words in abstracts, etc.

The Nuclear_refs_manager program package is written in C language and works on the operational systems Linux (X Window) and MS Windows. For more details see presentation (Annex 3).

2.3. ALPHAD-RADd and update of r0, Balraj Singh, McMaster University

The RadD code, which deduces r0 values for odd-A and odd-odd-A by interpolation of values for neighbouring even-even nuclides, was presented at the 2015 NSDD meeting in Vienna. It was suggested at the meeting to extend this code and merge it with the ALPHAD code. At the 2015 October IAEA-ENSDF-codes meeting, the first version of the new ALPHAD-RadD code was presented, which merged the previous ALPHAD code with the RadD code, but still using the 1998Ak04 (Nuclear Data Sheets 84, 1) Table of r0 values. During 2016-2018, the following tasks were carried out: 1. Improvement of original ALPHAD, by removing a couple of bugs in the code. 2. Large task of update of r0 values for all the 182 e-e alpha emitters, by incorporating revised half-lives, alpha branching ratios, alpha intensities to the ground states, and the Q(α) values from AME-2016 (Chin. Phys. C 41, 030003 (2017)). Finally, the ALPHAD-RadD code with the updated table was made available in April 2018 for testing by the network evaluators. Two main tables and systematics graphs were created for documentation and a paper was submitted for publication in the Nuclear Data Sheets. This paper contained the r0

parameter table for e-e alpha emitters, a table listing the relevant quantities used to obtain r0 values, and a systematics plot for all Z, as well as separate plots ordered by Z. A brief comparison of the new ALPHAD-RadD and the previous ALPHAD codes is as follows: 1. In datasets for even-even α emitters, a statement about deduced r0 parameter by assuming HF=1.0 for g.s. to g.s. α transition is automatically inserted in the data file by the ALPHAD-RadD code, whereas in the ALPHAD code, the insertion of deduced r0 is done manually in the dataset. 2. In datasets for odd-A and odd-odd-A α emitters, r0 is automatically deduced by the code, with the option that users are also prompted to provide r0 parameter of their choice. The statement for r0 parameter gets automatically inserted in the dataset, together with the deduced values of the alpha hindrance factors (HF), whereas in the ALPHAD code, r0 needs to be deduced manually following a certain recipe as given in M.J. Martin's memo, then edited in the input data file.

2.4. J-GAMUT code, Balraj Singh, McMaster University

At the June 2014 IAEA-ENSDF-codes meeting, a new code was proposed to: 1. automatize deduction of Adopted Gamma-ray energies and photon branching ratios from multiple datasets for a nuclide following a gamma-by-gamma approach, and 2. Revive the GAMUT code (R. Firestone: LBL-26024 (1991): A Computer Code for γ-ray Energy and Intensity Analysis) written in Fortran in the 80's, and rewrite it in a modern language such as JAVA. During Sept 2014 – Aug 2015: Michael Birch, in consultation with B. Singh, worked on this code and at the October 2015 IAEA-ENSDF codes meeting, he presented the new code, together with a simple example. Later this version was modified to correct for recoil energy as well as create an output file of Adopted Levels, Gammas in ENSDF format. In 2018, several other bugs came to attention, some through the network evaluators, but mainly from work on A=130 evaluation by Sorin Pascu (Bucharest) and B. Singh, where a large number of datasets needed to be analysed for ^{130}Xe and ^{130}Te nuclides. Most of these issues were in the GAMUT routine, but some also in gamma-by-gamma. For creation of Adopted datasets for gamma-ray energies and relative photon branching ratios for ^{130}Xe and ^{130}Te nuclides, both approaches i.e. gamma-by-gamma and GAMUT were used: GAMUT gives Eγ as level-energy differences, a departure from the general approach of recommending Eγ values based only on the measured gamma-ray energies. Finally, the Eγ values were taken from the gamma-by-gamma approach. With that approach, the level energies given by GAMUT were not quite consistent with Eγ values, thus the GTOL code was used to obtain level energies. Relative photon branchings were taken from the GAMUT analysis of the code. During the present meeting, the functioning of the code was tried at the NNDC as well as by B. Singh on several data files for nuclides with many datasets. It was found that the code stalled on a majority of these data files, without creating an 'intermediate file'. Michael Birch was contacted after the meeting, and he has agreed to look into the issue of stalling of the code. [Sec. note: Michael Birch has already been contacted, and he is working on modifications in the code, and also on the inclusion of some options for closely-spaced doublets, as suggested by B. Singh, with expected completion of this work by February 2019].

During the same period, Sept 2014 – Aug 2015, M. Birch also worked with B. Singh on rewriting the V_AVELIB in JAVA from its previous version in Visual-Basic. The asymmetric uncertainties in JAVA V_AVELIB code were handled following a modified version of the approach proposed by R. Barlow in arXiv:physics/0406120v1 (2004).

2.5. Java-RULER and ConsistencyCheck, Jun Chen, MSU (remote connection)

Java-RULER:

- written in Java with all functions as in the old Fortran version
- Solves issues with error propagations of large and asymmetric uncertainties

ConsistencyCheck:

- Main functions for checking:
  - Check data consistency among datasets (Adopted and individuals), e.g., JPI, MULT, XREF, T1/2, etc.
  - Check data validity (physics), e.g., large B(XL) compared to RUL, gammas with large ΔJPI, decay branches with large ΔJPI, etc.
- Functions for speeding up preparation of Adopted datasets:
  - Group ENSDF lines of levels and gammas (including comment lines) from individual datasets in one place for a quick view of all available data from different reactions
  - Average EG, RI and T1/2 with uncertainties in the same group and generate averaging comments in ENSDF that can be directly copied and pasted into the Adopted dataset (copy-and-paste is not automated since human evaluation is needed here)
- Other useful functions:
  - Setting up and creating evaluation folders when starting a new mass-chain evaluation
  - Sorting and merging individual datasets
  - Splitting a large file of multiple datasets into files of single dataset.

2.6. Codes development at ANL, Filip Kondev, ANL

The codes development work at ANL was focused on the existing RULER code, as well as on developing a new RULER code that deals with large symmetric and non-symmetric uncertainties.

The original Fortran RULER code has been modified to include the latest values of the fundamental constants. The subroutine that is used to calculate the Weisskopf partial lifetimes was also corrected. The logic of the error propagation of the individual gamma-ray branching ratios was modified to include the approach outlined by E. Browne (NIM A249 (1986) 461). Some other cosmetic changes were also made. The code was benchmarked with the stand-alone pyruler version and the results were found to be identical.

The stand-alone version of the RULER code, named pyruler, was completed. It is written in python and allows interactive input of data that are used to calculate the reduced gamma-ray transition probabilities. The uncertainties are propagated using the python uncertainties package (https://pythonhosted.org/uncertainties/). The pyruler results were compared to those produced by Jun Chen's java-code (java-ruler) and all were found to be identical in cases where the Taylor expansion assumptions are valid (e.g. for small uncertainties of the input quantities – in mathematical terms this means that the linear terms of the final calculated functions around the nominal values of their variables should be much larger than the remaining higher-order terms in the region of significant probability (because such higher-order contributions are neglected)).

Table 1: Comparison between java-ruler and pyruler codes for selected cases

	jruler	pyruler
100 keV, E1, RI=100	1.58 (8)E-6	1.58(8)E-6
100 keV, M1+E2, RI=100	M1: 3.4(6)E-5	M1: 3.4(6)E-5
δ=0.5(2)	E2: 0.37(24)	E2: 0.37(24)
71.64, E1+M2, RI=1.58	E1: 1.24(5)E-5	E1: 1.24(5)E-5
δ=0.018(9)	M2: 4 (4)	M2: 4 (4)
208.36, E1+M2, RI=89.3	E1: 3.17(8)E-5	E1: 3.17(8)E-5
δ=0.076(19)	M2: 19 (10)	M2: 19 (10)
321.31, E1+M2, RI=1.88	E1: 1.77(6)E-5	E1: 1.77(6)E-5
δ=0.175(10)	M2: 0.24 (3)	M2: 0.24 (3)

A new RULER code, named pyruler_MC, that uses the python Monte-Carlo mcerp package (https://pythonhosted.org/mcerp/) for propagation of the uncertainties was developed. mcerp is a stochastic calculator for Monte Carlo methods that uses latin-hypercube sampling to perform non-order specific uncertainty analysis. With this package one can easily and transparently track the effects of uncertainty through mathematical calculations. Advanced mathematical functions, similar to those in the standard python math module, can also be evaluated directly.

The pyruler_MC code treats cases properly where the uncertainties of the input quantities are symmetric and relatively large. In such cases the final uncertainties for the gamma-ray transition probabilities are often asymmetric. A version that will include treatments of the non-symmetric uncertainties and limits of the input quantities is currently under development. The results from the pyruler_MC code were compared (see Table 2) with those produced by the Jun Chen java-code (java-ruler), where upper and lower limits of the input quantities are used. It seems that the uncertainties estimated by the java-ruler code are overestimated compared to those produced by the pyruler_MC code.

Table 2: Comparison between java-ruler and pyruler_MC codes for selected cases

	jruler	pyruler_MC
71.64, E1+M2, RI=1.58 (5)	E1: 1.2(+10-5)E-5	E1: 1.2(+5-4)E-5
d=0.018(9)	M2: 4 (+11-3)	M2: 4(+5-3)
208.36, E1+M2, RI=100.0 (14)	E1: 3.1(+9-6)E-5	E1: 3.2(+13-9)E-5
d=0.076(19)	M2: 19 (+19-10)	M2: 19(+15-9)
321.31, E1+M2, RI=2.10 (4)	E1: 1.8(+15-8)E-5	E1: 1.8(+7-5)E-5
d=0.175(10)	M2: 0.24 (+25-12)	M2: 0.24 (+11-7)

2.7. Improvements in BetaShape, Xavier Mougeot, LHNB-Saclay

The first version of BetaShape, a new code for improved calculations of beta spectra, was released in 2016. The main features of this code include improved theoretical modelling of beta decay, a database of experimental shape factors, the provision of mean energies and logft-values, as well as beta and neutrino spectra, the ability to interface with ENSDF files, and the propagation of the uncertainties from the input data. A few months later, it was officially adopted by the DDEP (Decay Data Evaluation Project) international collaboration for future decay data evaluations.

The developments since then have been implemented in a new version of the code. The modelling of radiative corrections -based on a model developed in the 1970s-has been replaced by an accurate and modern model developed in the context of the high-precision study of super-allowed beta decays. In addition, the treatment of the uncertainty propagation has been modified for those cases where the uncertainty information is missing in the input file since the previous treatment led to unrealistic values. The database of experimental shape factors has been updated for the ^{138}La beta-minus transition, and the ground-state-to-ground-state beta-plus transition occurring in ^{14}O decay has been added. Following a request from different users who had difficulties in using the code, a specific file format compatible with the ENSDF format is proposed to directly provide recommended beta spectra in an ENSDF file. A continuation record is also proposed to provide the parameters of an experimental shape factor within the ENSDF file.

Electron capture transition properties are crucial features when evaluating the decay scheme of radionuclides. Pure electron capture radionuclides can be standardised using the TDCR-LSC method, whose uncertainty partly depends on the decay scheme. A precise knowledge of capture probabilities is also crucial for many applications such as dating rocks and fossils in geo- and cosmo-chronology; determining radiation effects on human tissues at the DNA level in nuclear medicine; or evaluating the background sources in fundamental physics experiments which measure rare events. An improved modelling of electron captures has also been developed starting from scratch, based on Behrens and Bühring's formalism. Allowed and forbidden unique transitions are calculated using relativistic wave functions of the atomic electrons, determined over the whole space in order to calculate overlaps of wave functions. The two common approaches from Bahcall and Vatai to correct for the atomic overlap and exchange effects have been extended to every subshell in a unified formulation, with the electron occupation treated precisely. The shake-up and shake-off effects, which create secondary vacancies, and the influence of the hole due to the capture process, have been considered. Uncertainties are also estimated. Relative capture probabilities and their ratios, including capture-to-positron ratios, are provided for each subshell. Additional ongoing developments will be presented at the next ICRM conference in 2019, in particular the influence of precise atomic orbital energies – determined using the Relativistic Local Density Approximation and taken from NIST website. These new developments are part of the European EMPIR project MetroMMC.

Another ongoing development is part of the European EMPIR project MetroBeta and is related to the inclusion of the nuclear structure component in the calculation of low-energy weak interaction decays. All the equations have been derived for beta minus, beta plus and electron capture transitions. The preliminary code developed in the last few months has been validated using simple nucleon wave functions determined from a naive shell model

considering both non-relativistic and relativistic harmonic oscillator solutions. Theoretical shape factors and partial half-lives of about twenty beta transitions, allowed and forbidden, have been calculated and compared to measurements. This work has to be considered as the very first step as only single particle nuclear matrix elements are calculated in spherical symmetry. However, it lays the foundations for future work for a correct treatment of deformed nuclei and forbidden non-unique transitions using nuclear wave functions from precise nuclear structure models.

A new version of the BetaShape code is expected to be released by June 2019, which will include the treatment of electron captures in a preliminary version for being tested by evaluators. Comments made during this Technical Meeting about the proposed format to include continuous spectra within ENSDF files will be taken into account (see below). The BetaShape code will be applied to all DDEP evaluations and the beta spectra associated with each evaluation will be made available on the newly developed LNHB website.

Proposed format for continuous spectra

This draft format would use the already existing Particle Record. Each continuous spectrum would have to be associated with its transition record, i.e. the Particle Record would have to follow the Beta Record in the case of a beta or antineutrino spectrum, the EC Record in the case of a positron or a neutrino spectrum, etc. Each line of the continuous spectrum would be a Continuation Record of the first Particle Record.

Additional symbols would be required in order to identify the particle in column 9:

- Existing: 'N' for neutron; 'P' for proton; 'A' for alpha.
- Additional: 'e' for electron; 'p' for positron; 'n' for neutrino; 'a' for antineutrino; 'g' for photon.

Then, the energy of the particle would be given in the appropriate field (columns 10-19) and the probability would be given in the intensity field (columns 22-29). Each spectrum would be normalized to unity in order to be scaled by the transition intensity, in accordance with ENSDF policies.

This format could also be used for providing electron capture probabilities and capture-to-positron ratios for all atomic subshells.

2.8. BrIcc Updates, Tibor Kibedi, ANU

The value of the total conversion coefficient CC is important to calculate total transition rates, normalization of level schemes, etc. In some cases, CC has been measured or determined from intensity balance and is placed into the G card: columns 56:62 holds CC and columns 63:64 its uncertainty, DCC. The total conversion coefficient is also calculated by BrIcc using Z, the transition energy, multipolarity and mixing ratio. The current practice is as follows:

- CC(DCC) – is the experimental value if it is known; "CC$" should be on G-comment record
- Calculated CC is provided for pure multipolarities, CC(DCC) for mixed transitions; DCC is also given if DCC/CC is large

This practice could lead to BrIcc overwriting the experimental CC by the calculated CC value. The following protocol was suggested and will be implemented in BrIcc:

a) If CC(DCC) is populated and G-comment card has “CC$” or “CC ” (c10:20), the put calculated CC(DCC) on S_G card
b) If the calculated CC(DCC) is different to CC(DCC) on the G-record, flag it in the calculation report
c) If CC(DCC) is blank or NO “CC$” in G-comment record, insert CC(DC) onto G-card

The current version of BrIcc does not calculate CC for mixed E0+E2+M1 transitions, however it calculates the CC value for a mixed E2+M1 transition, ignoring the E0 component. It was suggested not to calculate any CC value in these cases, but to flag them in the calculation report.

2.9. GABS update, Tibor Kibedi, ANU

The GABS code, written by E. Browne (LBNL), was designed to calculate the normalization coefficient (NR) and absolute γ-ray intensities (%RI) for 100 decays of the parent nucleus. The program also calculates the decay mode branching ratio (BR). It was noted that the uncertainties for γ-transitions used for the normalization are overestimated if not treated with the GABS approach. At the 21st NSDD meeting a proposal was adopted to put the %IG values provided by GABS in a continuation record to solve this problem.

The original GABS code has been significantly re-written to simplify the logical flow and to use input and output routines from the NSDFlib. The new code reads the complete ENSDF file that is stored in the memory. During the input most of the fields on the G, G-continuation and N records are tested for consistency and the program will stop if an error is detected.

GABS can now run interactively or by providing the input file and an option switch on the command line. GABS has 3 operation modes:

-F : GABS will calculate the NR normalization and BR branching factors and will produce the normalized gamma intensities, %GI".

-C : Using the NR, BR and NB (β-, β+, EC only) values from the N-record in the input ENSDF file, GABS will calculate the normalized %IG" intensities. A new report file is generated.

-M : The input file will be scanned to identify gamma transitions to the ground state. Transitions with non-zero DRI will be marked with ``X" in the 79th column. Transitions with blank DRI will be marked with ``Y". GABS will also calculate TI (if it was blank in the ENSDF input file) from RI and CC. Summed RI and TI values for all transitions going to the ground state will be listed. No output ENSDF _le will be generated.

It was also recommended at the codes meeting, that γ-ray transitions with blank DRI or DTI field should no longer be used in the normalization calculation.

The Program manual has also been re-written and now includes a comprehensive list of the normalization methods (originally described by J.K. Tuli).

The new version of GABS is expected to be released in January 2019.

2.10. BrIccEmis and NS_RADLIST, Tibor Kibedi, ANU

The BrIccEmis code, developed at the ANU [1], has been extensively used to calculate the emission spectra of X-rays and Auger electrons for a range of radioactive isotopes decaying

by electron capture and/or internal conversion [2,3,4]. At the last NSDD meeting in 2017, a proposal was accepted to include atomic data in decay data sets.

Progress has been made at the ANU to develop a new atomic radiation data base and a new code, NS_RadList to evaluate the X-ray and Auger electron yields, using ENSDF files as input nuclear data for the calculations. The program reads and verifies the complete data set using the newly developed NS_Lib library, then evaluates the distribution of primary atomic vacancies created in EC decay and/or internal conversion. In the final step the code generates the full atomic radiation spectrum and calculates mean energies, energy ranges and absolute transition rates for a number (~50) predefined Auger and X-ray groups according to the UIPAC notation: KLL, KLX, KXY, etc. for Auger electrons and KL2, KL3, KM, etc for X-rays. A comprehensive report file with a full list of gamma-rays, conversion electrons, Auger electrons and X-rays, an optional plot, using GnuPlot scripts, as well as new ENSDF records is also generated.

Considering the complexity of the calculations, involving a full Monte-Carlo treatment of the vacancy propagation, as well as the accuracy of the atomic transition probabilities in EADL, at this stage we do not propose to calculate the uncertainties of the atomic radiation yields.

A new ENSDF record type “M” has been accepted and representative new ENSDF records are shown below:

103RH AM E(Tot)= 0.416$ I(Tot)= 9.78E+02$

103RH2 AM E(Ktot)= 17.758$ I(Ktot)= 1.77E+00$

103RH2 AM E(KLL)= 16.857$ I(KLL)= 1.24E+00$

103RH2 AM E(KLX)= 19.627$ I(KLX)= 4.88E-01$

103RH XM E(tot)= 11.995$ I(tot)= 1.44E+01$

103RH2 XM E(Ktot)= 20.661$ I(Ktot)= 7.47E+00$

103RH2 XM E(KL2)= 20.134$ I(KL2)= 2.16E+00$

103RH2 XM E(KL3)= 20.279$ I(KL3)= 4.08E+00$

The development will continue through the first half of 2019. Extensive testing of the code is required, as well as implementing necessary changes to other codes to read the new atomic relaxation records.

A full publication of the BrIccEmis data base as well as the NS_Radlist is also planned before it`s public release later in 2019.

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[2] B.Q. Lee, et al., EPJ Web of Conferences 91 (2015) 7.
[3] M. Alotiby, et al. Physics in Medicine and Biology **63** (2018) 06NT04.
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2.11. UncTools, Tibor Kibdei, ANU

In ENSDF, a physical parameter is given in terms of a value with an optional physical unit as well as an uncertainty, which is usually the standard deviation. While most of the quantities fall under this category, some parameters (DFT, DMR, DT, DNB, DQA) could have asymmetric uncertainties. It is also possible, that a physical quantity is specified as a limit, or that it is known as a single assumed value. Using these parameters to derive other quantities, like mixed conversion coefficient, total intensity, intensity balance across an excited state, etc. requires the correct treatment of the uncertainties. Most of the ENSDF codes adopt the same analytical solution for error propagation, which is only valid for small relative and symmetric uncertainties. Combining a range of parameters in this same approach often leads to rather complicated procedures that result in errors, as has been shown in the well-known case of RULER.

A widely used method to propagate uncertainties is the Monte-Carlo approach [1]. Here each parameter is represented with a probability density function, PDF (symmetric, asymmetric normal distribution, squared distribution for limits, etc.) and drawing values from this PDF N times allows the repeated evaluation of a physical formula and the construction of the PDF of the output quantity. The PDF of the output quantity can be used to deduce the average (mean) value and it`s standard deviation. The coverage interval can also be determined. More studies are needed to revise the general policies for error propagation in ENSDF, including cases where the sampling may result in non-physical input or output parameter values (negative time, energy, conversion coefficient, etc.).

A new code, UncTools has been developed to propagate uncertainties through mathematical expressions. Parameter values and expressions are given in a script file, allowing to test a wide range of scenarios and values expected in the ENSDF evaluation work using the Monte-Carlo approach. The program uses the newly developed NS_Lib library and BrIcc to access conversion coefficients for the energies sampled during the Monte-Carlo calculations. Further tests will be carried out on the code, before it can be adapted to provide error propagation in other ENSDF codes, such as GABS, BrIcc, BrIccMixing, Radlist, Ruler, etc.

A sample input script to evaluate the B(E2) value in 122Cd and the graphical output are shown in Figs. 1 and 2.

```
# B(E2) from 122Cd; data from Table 3 of [2016r01]
# B(E2)[e2b2]=40.81E13*Eg**(-5){keV}/[(1+Icc_)*tau{s}]
# Param             Value     Unc    Mult
[G_1]  122Cd        569.45    8      E2
[G_1_CC_E2]                                          # from BrIcc
[tau]                15.4       +129-48                 # Mean life
time in ps
[G1_E]              569.45    8
[eqn] B(E2) = 40.81E13*G1_E**(-5)/((1+G_1_CC_E2)*tau) [plt]
```

FIG. 1 122Cd_BE2.unc input script.

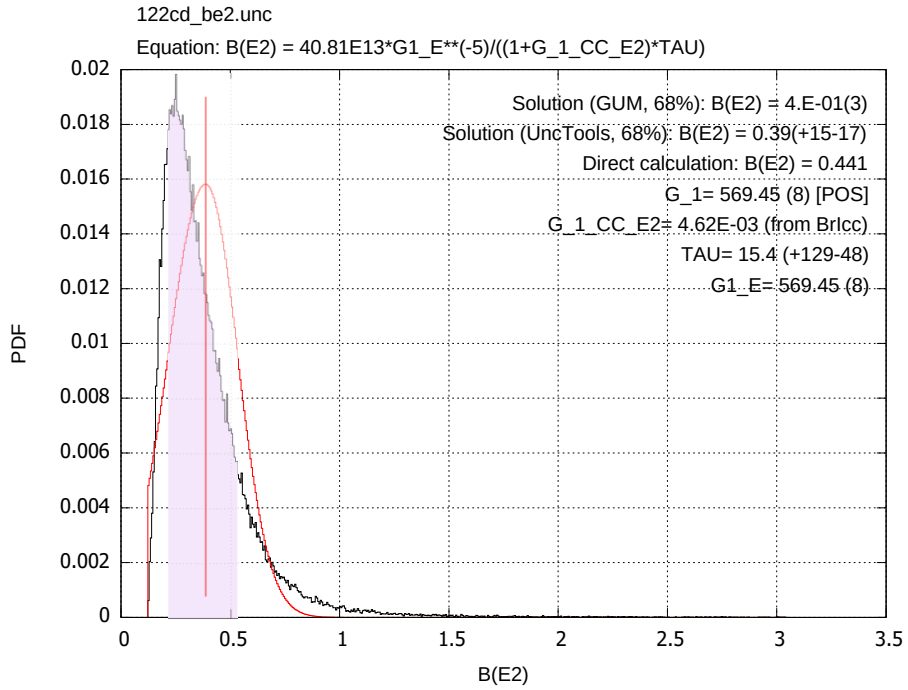

FIG.2 PDF of the B(E2) values evaluated with UncTools

Reference

[1] GUM, Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method, JCGM 101:2008

3. Technical discussions

Participants' presentations were followed by a detailed review of the priority table of codes that was produced in the previous meeting. Each code was discussed separately, and recommendations were made for further actions. The updated table is available in Appendix 2. A summary of the discussions for each code is presented in the following.

3.1. Editors and web tools

3.1.1. MyEnsdf Web tool

Some of the codes uploaded on this web tool need to be validated by evaluators:

NewGtol (PNPI): it is an extension of Gtol that treats singular matrices that cannot be handled by Gtol. A standalone version will be provided to B. Singh, F. Kondev, J. Tuli, and E. McCutchan for testing.

Action on V. Zerkin, M. Verpelli: to make available standalone versions of the codes NewGtol, Baron, and format checking codes developed at PNPI to the user community via the IAEA ENSDF Codes web page.

Java-NDS: V. Zerkin should work together with J. Chen to make Java-NDS run on MyEnsdf Web tool as the publication. NDSPUB will become an archival code.

IAEA Web editor (Zerkin): the tree editor with pop-up window editing developed so far, will be further developed to include additional editing functions. A working version will be presented at the upcoming NSDD meeting in April 2019.

3.1.2. NSR_refs_manager (PNPI)

The software runs on Linux and through virtual machine on Windows and MAC OS. The program allows the user to organise and manage any local collection of pdfs, image files, videos etc. The suggestion was to include capability to export search results to BibTeX (or Endnote) and import citations from NSR.

The program manager will be distributed to members of the NSDD network upon request.

3.1.3. NSR-PDF and X4-PDF database

An effort should be made to include conference proceedings that are made available on the web. The access to the database is restricted to compilers and evaluators collaborating with the IAEA. In the future, individual passwords should be issued.

3.1.4. GABS

A modified version of the code was presented by T. Kibedi, that searches for transitions to the ground state and calculates gamma-ray emission probabilities using the normalization factor provided in the ENSDF file. In addition, it creates a report file and a new ENSDF file with the absolute emission probabilities and their uncertainties inserted in the continuation record.

B. Singh suggested that in cases where the RI *field* is a limit, or CA or assumed, the transition will not be included in the GABS calculations. In addition, if DRI is blank or RI is AP, the user will be prompted to provide a value for the uncertainty.

Rounding off in ENSDF was also discussed. NDSLIB library does not follow ENSDF rules. Rule of 25 should be discussed again at the NSDD meeting.

The code will be tested by A. Sonzogni, F. Kondev, B. Singh, S. Basunia and E. McCutchan.

Deadline for distributing the beta version for testing is: 1 March 2019.

3.1.5. ALPHAD-RAdD

On MAC OSX the new code prints both the old and new r0 values. The new r0 tables are currently being checked.

The second beta version of the code will be distributed for testing on 1 March 2019.

It will be tested by F. Kondev, J. Chen, C. Nesaraja, and E. McCutchan.

The beta version of the code will be relocated to a section for codes ‘under development’ on the IAEA ENSDF Codes web page.

3.1.6. JGAMUT

The code has issues with level matching, as it has been found to run on some files but hang on many more files. B. Singh will discuss these issues with M. Birch and with J. Chen who has kindly agreed to maintain the code in the future.

The code will be relocated to a section dedicated to codes ‘under development’ on the IAEA ENSDF Codes web page.

3.1.7. V. AveLib

The code is stable and future maintenance will be the responsibility of J. Chen and B. Singh.

3.1.8. ConsistencyCheck (J. Chen): new code

The code has enhanced physics and consistency checking capabilities. It was recommended that it is distributed to the evaluators who should be encouraged to use it and provide their feedback and possible additional items to check to J. Chen, B. Singh and E. McCutchan.

3.1.9. Radlist codes

The legacy Radlist code (Burrows) has been reported to suffer from various bugs as well as physics limitations. As a result, one new Radlist code has been developed and a second one is under development within the network:

Web Radlist (Java code) (A. Sonzogni): It is a working code and therefore is the one that should be used by the network evaluators. It assigns numerical values to non-numerical uncertainties found in the ENSDF files. A note was made to include an advice to evaluators to avoid using non-numerical uncertainties in the decay data sets.

Some issues found in the code are going to be addressed by A. Sonzogni. Deadline for distributing a corrected working version is 1 March 2019.

NS_Radlist (T. Kibedi): calculates the gamma and conversion electron emission rates from nuclear decay, using ENSDF files as input. The program also calculates the complete Auger and X-ray spectra following EC-decay and internal conversion. These calculations are using the BrIccEmis database. It was suggested to evaluate the intensity of annihilation radiations from β^+ decay and electron-positron pair conversion. NS_Radlist requires some further development and will most likely be available for testing in a beta version in 6-7 months.

Another code that calculates atomic radiation starting from an ENSDF file using the same approach adopted in the Radlist/Emission code (Schonfeld) based on atomic data from Schonfeld, was developed at the IAEA (M. Verpelli) and is used to derive the atomic radiation data for LiveChart.

3.1.10. Ruler codes

The legacy Ruler code does not propagate uncertainties properly in cases when they are relatively large and does not treat asymmetric uncertainties either. The alternative approaches are:

Java-Ruler (J. Chen): **new code**. The code treats both large uncertainties and asymmetric uncertainties using the upper/lower limits.

Python Monte Carlo Ruler (F. Kondev): deals with both large uncertainties and asymmetric uncertainties using the Monte Carlo method.

NS_Ruler (T. Kibedi): uses the UncTools module to propagate uncertainties and is integrated with BrIcc to calculate conversion coefficients as needed. The code requires several months of development, therefore, until it is adequately tested, it was recommended that the network evaluators use Java-Ruler.

Python Ruler can be used independently to test these two other Ruler codes, Java-Ruler and NS_Ruler.

3.1.11. BetaShape

A new version of the BetaShape code is expected to be released by the end of 2018. This version will deal with bug fixes, new radiative corrections and will also include an updated experimental shape factors database. The treatment of missing or non-numerical uncertainties in the decay data set has also been modified to agree with the current Logft code. The format for continuous spectra discussed at this meeting (see Section 2.7) will also be adopted in this release of the code.

A preliminary version including the treatment of electron captures is expected to be made available by June 2019 for testing by evaluators. It will also produce as output continuous spectra in ENSDF files in the format agreed at this meeting.

The BetaShape code will be adopted in all DDEP evaluations and the beta spectra associated with each evaluation will be made available on the newly developed LNHB website.

3.1.12. Uncertainties in ENSDF

Blank uncertainties: the interpretation of blank uncertainty records in the ENSDF file is currently problematic, especially for the applications user community. Whether an uncertainty is unknown or zero should be easily distinguished in the file. There needs to be a clear policy that is implemented by all evaluators. Such a policy should be discussed at the upcoming NSDD meeting.

Asymmetric uncertainties

The Unctools was developed by T. Kibedi to propagate uncertainties based on a Monte Carlo approach. It was agreed that the Monte Carlo approach using Probability Density Functions allows propagating uncertainties in calculations of transition strengths, hindrance factors, absolute intensities, coefficients and atomic radiations, consistently as it deals with both small and large uncertainties as well as asymmetric uncertainties.

Especially in the case of the Ruler code, the proper treatment of large and asymmetric uncertainties is important for obtaining correct results. It was agreed that it would be useful to discuss the issue with expert(s) on treatment/handling of large and asymmetric uncertainties of experimental data, possibly from the metrology community and/or particle data group.

A recommendation was made to the IAEA to organise a short meeting among ENSDF evaluators and these experts prior to the NSDD meeting in April 2019.

3.1.13. Extending the ENSDF format

Atomic radiation data (T. Kibedi):

The format that was endorsed at the previous NSDD meeting to include atomic radiation data in ENSDF was reviewed. Some additional changes were suggested.

The format will be checked by ENSDF manager (E. McCutchan) against the ENSDF manual and dictionaries and, whatever changes are required, will be implemented and presented at the NSDD meeting.

Continuous data (beta spectra, neutron spectre etc) (X. Mougeot/A. Sonzogni):

A proposal for a format to include continuous spectra in ENSDF was presented by X. Mougeot (see Section 2.7). It was extended to include all types of continuous particle spectra produced by beta- and beta+/EC decays. The proposed format will be scrutinized and checked against the ENSDF manual and dictionaries, FMTCHK and Java-NDS, with ENSDF manager (E. McCutchan) and T. Johnson, J. Chen, A. Sonzogni.

The proposal to include experimental shape factors for electrons and positrons as well as for EC probabilities to all the relevant sub-shells in the continuation record in ENSDF was discussed (see Section 2.7 and presentation of X. Mougeot in Annex 3). The advantages of including them were emphasized and a report will be presented at the NSDD meeting. Again, the proposed format will have to be checked by the ENSDF manager (E. McCutchan).

One more modification in the ENSDF format that will be proposed at the NSDD meeting by NNDC is in the Q record. The current Q record has certain limitations. It will therefore be proposed that the current Q record is accompanied by a continuation record that will accommodate certain Q values, separation energies and other relevant channels.

3.1.14. ENSDF Manual

NNDC has committed to updating the manual and cleaning up the continuation records. A list of recommended, new and obsolete continuation records will be produced and distributed to the network.

An updated version will be circulated on 1 March 2019. The plan is to revise the manual on a yearly basis.

3.1.15. Dissemination of codes

In the future, the ENSDF analysis and checking codes will be made available to the users from the NNDC upon request and submission of registration form that will certify that the user agrees and accepts the content of the disclaimer. One possible repository is GitHub. In general, it was agreed that password-controlled access to the codes is a safer way of dissemination.

In addition to the annual USNDP meetings at BNL, a meeting focussed on ENSDF analysis and checking codes will be organised at TUNL depending on the needs. This meeting will be open to evaluators and network members working on development of codes.

4. Perspectives

The perspectives for code development and maintenance within the network in the future were discussed. The NNDC plans to enhance its groups expertise and capabilities to maintain and develop the ENSDF Analysis and Checking codes. This plan is welcomed by the members of the network as the codes are essential tools in the evaluation procedure and therefore need to be reliable and up-to-date with physics models and evaluation procedures and policies.

In this respect, increased collaboration with LHNB-Saclay on analysis codes and evaluation is also encouraged.

The IAEA will continue to disseminate the ENSDF Analysis and Checking codes as long as deemed necessary. There was a proposal to include a separate section for codes under development or testing on the IAEA ENSDF Codes web page so that evaluators could try them and provide feedback. The complete list of actions agreed at the meeting is presented in Table 1.

APPENDIX 1

Table 1. List of Actions

#	Person	Action	Deadline
1	IAEA (V. Zerkin, M. Verpelli)	Make available standalone versions of the codes NewGtol, Baron, and format checking codes developed at PNPI to the user community via the IAEA ENSDF Codes web page	January 2019
2	IAEA (M. Verpelli)	Create separate section for codes under development or testing on the IAEA ENSDF Codes Web page	December 2018 - done
3	T. Kibedi	Distribution of beta version of new GABS code	1 March 2019
4	IAEA (V. Zerkin), J. Chen	Make Java-NDS run on MyEnsdf Web too	After meeting - done
5	B. Singh S. Singh	Distribution of 2nd beta version of ALPHAD-RaDd code	1 March 2019
6	NNDC (A. Sonzogni)	Distribution of corrected Web-Radlist code	1 March 2019
7	T. Kibedi	Include pair conversion and annihilation in atomic radiation records	1st March 2019
8	E. McCutchan T. Kibedi	Check Atomic Radiation format against the ENSDF manual and dictionaries and present whatever changes are required at the NSDD meeting	NSDD meeting (8-12 April 2019)
9	E. McCutchan, J. Chen, T. Johsnon, A. Sonzogni	Check new 'spectra' format against the ENSDF manual and dictionaries, FMTCHK and Java-NDS	NSDD meeting (8-12 April 2019)
10	NNDC (E. McCutchan, A. Sonzogni)	Update ENSDF Manual	1 March 2019
11	X. Mougeot	Beta version of BetaShape including EC	1 June 2019
12	IAEA (P. Dimitriou)	Recommendation: Organize a short meeting with experimental uncertainties experts and ENSDF evaluators to discuss error propagation methods	tbd

APPENDIX 2

Table 2. Review of Analysis Codes from previous meeting (INDC(NDS)-0696)

CODE	TASK	NAME	TIMELINE	PRESENT
JAVA NDS	FURTHER DEVELOPMENT AND TESTING	CHEN, SINGH	BETA-VERSION END OF NOVEMBER 2015	OFFICIAL PUBLICATION CODE
JGAMUT	IMPROVEMENT AND TESTING	BIRCH, SINGH	BETA VERSION END OF NOVEMBER 2015	DONE + RECOIL CORRECTIONS: VALIDATION: ISSUES WITH LEVEL ENERGY MATCHING MAINTENANCE
VISUAL AVERAGING LIBRARY	INCLUDE BARLOW METHOD AND PLOTTING	BIRCH, SINGH	END OF NOVEMBER 2015	DONE: MAINTENANCE: (J. CHEN)
BETASHAPE	IMPROVED TREATMENT OF FORBIDDEN NON-UNIQUE + EC	MOUGEOT	JANUARY 2016 NEXT CODES MEETING	DONE VALIDATION OF LOGFT ONGOING
EDITOR	EXPLORE DIFFERENT OPTIONS	ZERKIN	IN PROGRESS- ZERKIN TO START END OF SUMMER 2016	ENSDF± AVAILABLE DEVELOPMENT ONGOING

APPENDIX 2

CODE	TASK	NAME	TIMELINE	PRESENT
R0 (RADd) CODE	INCORPORATION IN ALPHAD	SINGH, SINGH	IN PROGRESS FEBRUARY 2016	DONE: NEW ALPHAD-RAdD CODE TO BE VALIDATED NEW R0 TABLES – TO BE PUBLISHED
NEW R0 TABLES	UPDATE R0 TABLES FOR NEW Q-VALUES, BRANCHINGS AND NUCLIDES	SINGH, SINGH		
ONLINE WEBTOOL	MAKE PNPI CHECKING CODES AVAILABLE	ZERKIN	MID-2016	DONE
PANDORA	ENHANCE CODE	TULI-NSDD NETWORK	CONTINUOUS	BAND ASSIGNMENT (ZERKIN) MAINTENANCE WTH NNDC
FMTCHK	ENHANCE FORMAT CHECKING	NNDC INVOLVE PNPI GROUP	CONTINUOUS	NNDC (JOHNSON) CONTINUOUS BUG FIXES DEVELOPMENT

APPENDIX 2

CODE	TASK	NAME	TIMELINE	PRESENT
NS_RULER PYRULER	DEVELOPMENT DEVELOPMENT AND TESTING	T. KIBÉDI, F. KONDEV, M. BIRCH	BETA VERSION BY JUNE 2016	ONGOING – TREATMENT OF ASYMMETRIC UNCERTAINTIES WITH MONTE CARLO AVAILABLE
NS_LIB	DEVELOPMENT AND TESTING	T. KIBÉDI	NEXT CODES MEETING	DONE
BRICCEMIS/ NS_RADLIST	DEVELOPMENT	T. KIBÉDI	IN PROGRESS REPORT AT NEXT CODES MEETING	ONGOING – ASYMMETRIC UNCERTAINTIES WITH MONTE CARLO
LOGFT	WARNING MESSAGES FOR UNPHYSICAL INPUT DATA AND ASSIGNMENT OF UNCERTAINTIES	NNDC	PENDING	TO BE REPLACED BY IMPROVED CODE IN FUTURE (BETASHAPE AFTER VALIDATION)

ANNEX 1

Technical Meeting on

"Improvement of Codes for Nuclear Structure and Decay Data Evaluations"

IAEA, Vienna, Austria
3-7 December 2018
Meeting Room VIC MOE24

ADOPTED AGENDA

Monday, 3 December

08:30 – 09:00 **Registration (IAEA Registration Desk, Gate 1)**

09:00 – 09:30 **Opening Session**

Welcoming address (A. Koning)
Administrative matters
Election of Chairman and Rapporteur
Adoption of the Agenda

09:30 – 17:00 **Codes session I** – ***WebEx with J. Chen from 16:30***

1. Review of actions from previous meeting (2015): P. Dimitriou
2. Editors and web tools:
    a. MyEnsdf and ENSDF editor; V. Zerkin
3. NSR_refs_manager: package to manage NSR bibliography; A. Rodionov
4. GABS; T. Kibedi
5. Java-NDS: with participation of J. Chen (*WebEx at 16:30*)
    a. Feedback; A. Rodionov
    b. Inclusion on MyEnsdf Web tool; V. Zerkin

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Tuesday, 4 December

09:00 – 17:30 **Codes session II (cont'd from I) – *WebEx with J. Chen from 15:00***

6. ALPHAD-RAD and update or r0 parameter; B. Singh
7. JGAMUT:
    a. corrections and example; maintenance issue; B. Singh
    b. Feedback; A. Rodionov
8. V. AveLib: maintenance issue; B. Singh
9. BetaShape: new update; beta shape factors in ENSDF and beta spectra; X. Mougeot
10. Radlst codes:
    c. NNDC Radlst code; A. Sonzogni / E. McCutchan (*WebEx*)
    d. BrIccEmis-Radlst; T. Kibedi
    e. Atomic radiations code; M. Verpelli
11. Ruler codes: (*WebEx from 15:00*)
    f. Java Ruler; J. Chen (WebEx)
    g. T-Ruler; T. Kibedi
12. ENSDF Consistency check; Jun Chen (WebEx from 15:00)

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

19:00 **Dinner at a restaurant downtown**

Wednesday, 5 December

09:00 – 17:00 **Codes session III (cont'd from II) – *WebEx with J. Chen from 15:00***

13. Asymmmetric uncertainties: how to treat them in ENSDF evaluations
    a. Monte Carlo-PDF; Tibor Kibedi
    b. Stand-alone Monte Carlo; Filip Kondev
    c. Upper/lower limits; Jun Chen/Balraj Singh (Java-Ruler)
14. Validation of codes: how? Who? ALL
    a. General
    b. BetaShape
    c. JGAMUT
    d. GABS
    e. Java-Ruler
    f. Consistency-check

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Thursday, 6 December

09:00 – 17:00 **Codes session IV (cont'd from III) –** ***WebEx with J. Chen form 15:00***

15. New formats in ENSDF: proposals from 22nd NSDD 2017; update
    a. Atomic radiation data; T. Kibedi
    b. Continuous spectra; A. Sonzogni / X. Mougeot
16. Dissemination: update on status and future procedure
17. Perspectives

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Friday, 7 December

09:00 – 12:30 **Drafting of the Summary Report (cont'd)**

Closing of the Meeting

Coffee break(s) as needed

ANNEX 2

Technical Meeting on the Improvement of Analysis Codes for Nuclear Structure and Decay Data Evaluations

3 to 7 December 2018
IAEA, Vienna

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Links to Presentations

#	Author	Title	Link
1	P. Dimitriou	Review of Actions from ENSDF Codes Meeting 2015	PDF
2	V. Zerkin	MyEnsdf and ENSDF Editor	PDF
3	A. Rodionov	NSR_refs_manager package	PDF
4	J. Chen	Java-Ruler, ConsistencyCheck	PDF
5	V. Zerkin	Java-NDS on MyENSDF	PPT
6	B. Singh	ALPHAD-RAdD code	PDF
7	B. Singh	JGAMUT code	PDF
8	X. Mougeot	BetaShape code, beta shape factors and beta spectra in ENSDF	PDF
9	F. Kondev	RULER code	PDF
10	T. Kibedi	Uncertainty propagation tools	PDF
11	T. Kibedi	BrIcc - changes	PDF
12	T. Kibedi	Gabs v12	PDF
13	T. Kibedi	BrIccEmis and NS_RadList	PDF

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