IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Summary Report of 2nd Technical Meeting

Improvement of Analysis Codes for Nuclear Structure and Decay Data Evaluations

IAEA Headquarters, Vienna, Austria

5 - 8 October 2015

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Abstract

A summary is given of a Technical Meeting assembled to monitor progress in the effort to improve the analysis and utility codes used in the evaluation of nuclear structure and decay data for the Evaluated Nuclear Structure Data File (ENSDF). Participants discussed the new codes that were submitted for testing prior to the meeting, as well as the status of the remaining codes that are under development. Emphasis was placed on defining procedures for treating asymmetric uncertainties uniformly in all the new codes. Three alternative solutions for developing an evaluation toolkit were proposed, procedures for validating the codes were outlined and requirements for dissemination were recommended in the form of guidelines. The list of priorities of codes was revised and assignments were modified accordingly. Details of the discussions are presented in this report.

November 2015

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1. INTRODUCTION

The IAEA Nuclear Data Section (IAEA NDS) as coordinator of the international network of Nuclear Structure and Decay Data Evaluators (NSDD) has initiated a coordinated activity to address the problem of improvement and maintenance of analysis codes used for the evaluation of nuclear structure and decay data. The first Technical Meeting of this project was held from 10 to 13 June 2014, at the IAEA Headquarters in Vienna. Participants reviewed the status of all the analysis codes, identified the improvements that need to be made, outlined the general requirements for developing new codes, and produced a priority list of codes that need to be addressed. All the details of the discussions and the tasks assigned can be found in the summary report of that meeting INDC(NDS)-0665.

In this second Technical Meeting that was held from 5 to 8 October 2015, at the IAEA Headquarters in Vienna, participants discussed the progress of the project, re-assessed the status of the codes and the emerging data needs, and finally revised the list of assignments.

On the first day of the meeting, participants from Australia, Canada, France, India, Russian Federation and USA (see Annex 2 for Participant's List) were welcomed to the IAEA by the Scientific Secretary of the NSDD network and project, Paraskevi Dimitriou, who described the motivation and goals of the meeting. Jagdish Tuli (BNL) was elected chairman of the meeting, and Tibor Kibédi (ANU) agreed to act as Rapporteur. The meeting's Agenda was then adopted without changes (see Annex 1) and the meeting began with participant's presentations (summaries are included in Section 2 and links to the presentations in Annex 3).

2. PRESENTATIONS

Summaries of the presentations given at the meeting are provided in the following sections.

2.1. A contribution from the ANL Nuclear Data Program, F.G. Kondev (Argonne National Laboratory (ANL))

A report was given on the development of a stand-alone version of the RULER code, named pyRULER. It is written in python and allows interactive input of data that are used to calculate the reduced transition probabilities in nuclei. The uncertainties are propagated using the python *uncertainties* package. The treatment of non-symmetric uncertainties was also discussed and an implementation of the Monte-Carlo *mcerp* package was demonstrated. The distribution of the code is expected in early 2016.

2.2. JGAMUT: ENSDF Adopted Levels, Gammas Assistant Code – Summary, M. Birch (McMaster University)

A new code called "JGAMUT" has been written and the Visual Averaging Library (V.AveLib) code has been re-written in Java. The presentation summarized these codes as well as demonstrated their usage.

The Visual Averaging Library (V.AveLib) code includes 3 outlier detection methods and 8 different averaging methods. A modification to the algorithm used to calculate the average using the bootstrap method has been made from the original V.AveLib. This modification

greatly reduces the runtime of that method. In addition to being cross-platform, the advantage of re-writing this code in Java is that all the averaging methods are now easily used within the new JGAMUT code.

The motivation for creating JGAMUT was to make producing an Adopted Levels, Gammas (ALG) dataset less labour-intensive for evaluators, more standardized between different evaluators and allow for more sophisticated statistical methods to be used. The algorithms of JGAMUT fall into the following categories: parsing ENSDF input, gamma-by-gamma averaging, linear systematic energy shift calculation, the GAMUT energy algorithm and the GAMUT intensity algorithm.

The parsing of ENSDF input algorithm also must match the levels between different datasets which are the same. This algorithm is known to not be particularly robust and requires improvement.

The gamma-by-gamma averaging algorithm automates the procedure currently done by many evaluators. For each gamma-ray, measurements of its energy are averaged together and measurements of its intensity are also averaged together. The usual weighted average is used for consistent data, the normalized residuals method (NRM, as implemented in V.AveLib) is used for somewhat discrepant data and finally the unweighted average is used for very discrepant data.

The linear systematic energy shift algorithm is designed to detect calibration differences between different experiments. In this algorithm the evaluator chooses a "standard" dataset, which he or she believes is accurate and the code determines shifts relative to the standard based on least-squares fitting. Applying such shifts can improve the quality of the gamma-by-gamma averages if there are indeed systematic differences between different experiments.

The GAMUT energy algorithm (based on the algorithm used in the original GAMUT code by R.B. Firestone (LBNL) [LBL-26024 (1991)] determines the level energies using a least-squares fit to the level scheme. The adopted gamma-ray energies are then determined by level energy differences. This algorithm also allows for constant systematic shifts to be fitted (but this is unnecessary if the linear shifts above were already used).

The GAMUT intensity algorithm (based on the algorithm proposed by Tepel and Lederer [IAEA report INDC(NDS)-115/NE (1980)]) determines gamma intensities level-by-level through a χ^2 minimization procedure. For a fixed level, the measured intensities for different experiments are assumed to be related by scale factors, α_j. These scale factors and fitted intensities, $\bar{I}_i$, are determined by minimizing $\chi^2 = \sum_i \sum_j \frac{(I_{ij}\alpha_j - \bar{I}_i)^2}{(\alpha_j \Delta I_{ij})^2}$, where the first sum is over all gamma-rays depopulating the level and the second sum is over all measurements of that gamma's intensity. This minimization is done with the constraint that $\sum_i \bar{I}_i = 1$ so that the fitted intensities correspond to the branching ratios of the gamma-rays for that level.

2.3. Status of JAVA-NDS Computer Code for ENSDF-formatted Data Files, Jun Chen (NSCL, MSU) and Balraj Singh (McMaster University)

At the previous codes meeting (see web page), the topic of McMaster-developed JAVA-NDS computer code was brought up in discussions about an improved Web display of ENSDF data files.

Background: JAVA-NDS is a platform-independent code, which the ENSDF evaluators could use to generate their own manuscripts for Nuclear Data Sheets (NDS) journal. It was initiated by B. Singh in 2007, who suggested that his student Roy Zywina should write such a code in JAVA. With a contract from NNDC, BNL, and regular consultations with B. Singh, Roy worked during 2007-2008, and handed over a large, but inoperable code in early 2008, after which he quit in the middle of the contract.

In 2008-2009, B. Singh's student Scott Geraedts worked on this code to produce band drawings for NDS journal, and in 2009 a package to produce such drawings and insert pages in NDS publications was prepared and handed over to Marion Blennau at NNDC, BNL, which she used during 2009-2014 for several mass-chain publications in NDS. During 2009-2011, Scott and B. Singh's student Jeremie Choquette worked further on this code to produce complete tables and drawings of mass chains.

Operating versions of this code, with a control file for optimum layout of tables and drawings, were presented by B. Singh at NSDD-2009 and NSDD-2011 meetings. Tables and Drawings copies of complete mass chains A=182 in 2010 and A=75 in 2011 were produced in the style of Nuclear Data Sheets publications; the A=182 was checked in detail by several ENSDF evaluators for complete and accurate transcription of data, while A=75 was sent for review. Since 2013, Marco Verpelli at IAEA-NDS has been using this code for LiveChart of nuclides. However, for the purpose of NDS publications, the code still needed additional work to make it stable and more user-friendly. At the NSDD-2015 meeting held in April 20-24, 2015 in Vienna, in consultation with Jun Chen, B. Singh gave a presentation about this code, a working demonstration for A=43, and items for improvement of the code. Based on subsequent discussions at the meeting, Jun Chen started working on improving the 2011 version of the code in April 2015.

Brief description: JAVA-NDS code converts ENSDF-formatted data files to LaTeX; it uses LaTeX table and figure environments and MetaPost to generate drawings; it produces a script file to run LaTeX to produce a final output in PDF. The 2011 version used an editable control file for optimum layout of Tables and Drawings; generating this control file for a mass chain took 6-8 hours, a somewhat cumbersome process.

Progress from April-Sept 2015: As described in the presentation by B. Singh (see Annex 3), Jun Chen has made major modifications in the code, so that most of the settings are now made automatically by the program based on table positions and dimensions. There is still an option for manual setting with a control file for fine-tuning of the final layout of individual datasets or a published version. A single step through a graphic user interface (GUI) produces a final PDF output with automatic table orientation and table breaks. A long table is divided to sub-tables that only show in one page based on table position and page size; page breaks are inserted into the output LaTeX file by the program. Table orientation (portrait or landscape) is automatically set by the program based on estimated physical table-width in the PDF output. For long and narrow tables, table splitting and break points are determined automatically by the program based on table position, table size, and/or page size. The program scans the whole table and estimates the physical table size in the PDF output.

Further improvements to the code were discussed at this meeting. Jun Chen and B. Singh will check for stable working of the code during October-November 2015. The plan is to make the code available by the end of November 2015 as a beta version for testing by the NSDD network evaluators. At this meeting presentation, it was also suggested that JAVA-NDS outputs could be used either in PDF or some other format for Web display (on NNDC website or elsewhere) of ENSDF and XUNDL data files, while noting the persistent technical problems (such as waiting time, missing data, etc.) with the current Web-trend display in html format.

2.4. Improvement of analytical calculations of beta spectra, X. Mougeot (Laboratoire National Henri Becquerel-CEA)

Following the recommendations from the previous Technical Meeting on Improvement of Analysis Codes for Nuclear Structure and Decay Data Evaluations (summary report INDC(NDS)-0665), a program dedicated to the calculation of beta spectra has been developed with the ultimate intention of broadly disseminating it within the nuclear data evaluator community. To ensure fast computation and produce an easy-to-use program, it was decided not to include the fine atomic effects (exchange, new screening correction) which were presented at the previous meeting.

The present code is almost an analytical version of the BetaShape program. The calculations are performed using Behrens and Bühring formalism. Allowed and forbidden unique transitions are calculated without any limitation on the transition order, while forbidden non-unique transitions are determined using the ξ approximation. The Fermi function and the λ_k parameters involved in the definition of the theoretical shape factor are determined from the Coulomb amplitudes of the relativistic electron wave functions. These wave functions are calculated for the Coulomb potential of a uniformly charged sphere, which means that the finite nuclear size effect is intrinsically taken into account. As no analytical solution exists even for such a simple potential, Dirac equations are solved numerically according to *the fast, but complicated, method* of Behrens and Bühring [2.4.1]. The neutrino spectrum that corresponds to the beta spectrum is also calculated.

The Rose screening correction and the radiative corrections are considered exactly the same way as described in previous meeting. It is noteworthy that the radiative corrections for neutrinos are slightly different than for the electrons. A screening correction adapted from Bühring [2.4.2] was also implemented. The calculations are somewhat slower than for Rose screening, but Bühring screening exhibits no breakdown at low energy and is theoretically more refined. Most of the formalism, except for the Bühring screening correction, has been described in a recent publication [2.4.3] which also includes systematic comparisons of these calculations with a database of experimental shape factors.

This formalism was implemented within C++ classes and two interfaces were developed. The first one, called *bsan*, performs the calculation of a specific beta transition defined through input parameters and provides an output file with many details about the calculation, the experimental shape factor if found in the database, the mean energies of the spectra and some analysis parameters. The second interface, called *bsan_mult*, is dedicated to the calculation of multiple beta transitions from the decay of a specific radionuclide. Input parameters are determined from the nuclear data given in the ENSDF file of the radionuclide. Each individual transition is calculated through *bsan* and the total spectrum is built with each single spectrum normalized to its branching ratio. In addition to the individual output file of each transition, another output file provides the total spectra and many additional details. The individual spectrum constructed from the experimental shape factor is always preferred, if such is available.

The current code has been tested and works well for the 130 tabulated transitions of the database and for a very limited number of ENSDF files generated with Saisinuc (^{11}C, ^{40}K, ^{60}Co, ^{68}Ga, ^{75}Ge, ^{241}Pu). Extensive testing using ENSDF files obtained directly from the ENSDF database is required. The calculation of the log *ft* values and the propagation of the uncertainties from the input parameters still need to be carefully examined and implemented.

References

[2.4.1] H. Behrens, W. Bühring, *Electron Radial Wave functions and Nuclear Beta Decay*, Oxford Science Publications (1982).

[2.4.2] W. Bühring, *The screening correction to the Fermi function of nuclear β-decay and its model dependence*, Nuclear Physics A 430, 1 (1984).

[2.4.3] X. Mougeot, *Reliability of usual assumptions in the calculation of β and ν spectra*, Physical Review C 91, 055504 (2015).

2.5. NS_lib subroutine library, Tibor Kibédi (Australian National University)

We are developing a new subroutine library to support the ENSDF analysis codes, BrIcc, BrIccMixing, TRuler, TGabs, etc. The library is developed using Fortran 90. The core part of the library contains high-level routines to read, write, parse and validate complete ENSD data sets. The declaration of ENSDF data cards (Level, Gamma, Electron-Capture) with an extensive range of related other parameters are encapsulated into a single Fortran 90 module, NS_libMod.

A basic ENSDF parameter is declared as a derived Fortran 90 data type. This allows storing values in character and numerical form together with their uncertainty. The uncertainty field can be empty (no uncertainty), symmetric or asymmetric values, limits, etc. Single integer flags, set by the validation routines, to signal are used to signal incorrect or invalid values.

The current version of the development code can read parse and validate the complete ENSDF distribution file, more than 2 million lines in length, in less than a minute. The extensive validation routines are designed to carry out format as well as physics testing. Nearly one thousand error and warning messages have been defined to provide uniform feedback to the program users.

Future developments of the library will include program modules for error propagation using Monte Carlo methods. This will be a major step forward to improve the quality of the data mining capabilities of the ENSDF codes.

2.6. Revised ALPHAD (ALPHAD+RadD), Sukhjeet Singh (Maharishi Markandeshwar University Mullana)

The RadD code [2.6.1] was developed for deduction of the radius parameter (r_0) for input in the ALPHAD code. Subsequent to feedback received at the 21st NSDD meeting at IAEA, Vienna in April 2015 (summary report INDC(NDS)-0687), and follow-up discussions and comments during the Specialized Workshop the week after (summary report INDC(NDS)-688), it was decided to merge the RadD code into the existing ALPHAD code [2.6.2] . In order to keep the originality of ALPHAD, the RadD code has been appended as a subroutine in the ALPHAD main source code with its own input variables and with the same output variables namely, *fermi* and *dfermi*, used in existing ALPHAD code. This revised code has been tested for 20 different data sets of odd-odd and odd-A nuclei.

Further improvement of the ALPHAD+RadD code: In order to make the revised ALPHAD code more user-friendly, the following features are planned for inclusion:

1. For even-even nuclei: The RadD subroutine should not be called in the main program and the program execution should be directed to the original ALPHAD code.

2. For odd-A or odd-odd nuclei: If r_0 is provided by a user/evaluator, then that r_0 should be used along with the original ALPHAD code to deduce Hindrance Factors (HFs), otherwise r_0 should be deduced using RadD, followed by deduction of HFs using this deduced r_0 value.

3. For odd-A or odd-odd nuclei: While deducing the radius parameter using RadD, there may be   situations when either one or both of the input radius parameter(s) may not be available in Akovali's evaluation [2.6.3]. In such cases, a warning message will appear before the code terminates.

4. For even-A and Odd-A nuclei: The r_0 value used in the deduction of HFs should be listed in the output file as well as in the report file produced by the revised ALPHAD code.

Inclusion of above features in the revised ALPHAD package is expected by March 2016.

Update of Akovali's r_0 Table [2.6.3]: The 1998 tabulation of r_0 parameter for all known even-even alpha emitters is being updated for new Q(alpha) values, half-lives, branching ratios, and newly discovered even-even alpha emitters. This major undertaking is currently in progress, with expected completion date February 2016.

References

[2.6.1]   Sukhjeet Singh *et al*., (2015): *RadD*
           (http://www-nds.iaea.org/public/ensdf_pgm/index.htm)
[2.6.2]   http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/alphad/
[2.6.3]   Y. A. Akovali, Nuclear Data Sheets 84, 1 (1998).

2.7. G-forge for ENSDF and suggested improvements in FMTCHK and PANDORA codes, J. K. Tuli (NNDC-Brookhaven National Laboratory)

NNDC maintains the commercial software G-forge. It helps tracking codes, databases, and related correspondence. It helps with the versioning for codes and databases. It was suggested that all NDS evaluators should have access to ENSDF and its analysis code projects. NNDC has already provided such accounts for the participants of the current code meeting and other evaluators can get the accounts on request. G-forge would keep records for all the bugs, suggestions and comments and track their status and ultimate resolution. The codes, as well as, databases can be exchanged through G-forge and it will provide proper versioning.

The analysis program FMTCHK is the most used program and is needed at every stage an ENSDF-formatted file is created or modified. The program needs continuous maintenance to keep in synch with accepted changes in format and/or physics. It should also be user friendly and not put out too many unnecessary warnings.

The program PANDORA is one of the few physics checking programs for the evaluators and reviewers. Suggestions are welcome from the evaluators, and other users to expand its scope and include additional checks. Some modifications, like checking between the decay datasets and adopted are already contemplated. It was also suggested that it should provide a list of gamma rays feeding a given level, as well as the properties of the initial level depopulated by a given gamma ray. Any volunteers to modify the code are welcome.

2.8. Progress in MyEnsdf - web tools for ENSDF evaluators, V. Zerkin (NDS IAEA)

NDS web server calculation systems (MyEnsdf is one of them) allow the user to upload, test and process input data without the installation and configuration of codes. A user-friendly web interface and pre-loaded (ready-to-run) examples are available to help the user learn how to run all the nuclear data processing codes.

MyENSDF

http://www-nds.iaea.org/exfor/myensdf.htm

The system allows the user to run a number of codes emulating the terminal output as the user would see when running them locally: FMTCHK, chk_ENSDF, PREPRO, XPQCHK, ALPHAD, GTOL, BrIcc, BrIccMixing, GABS, LOGFT, PANDORA, RADLST, RULER, NDSPUB.

Recent progress:

- Added codes: ALPHAD, XPQCHK, RULER, GABS
- New features: sorting (by names, extensions, time, etc.); saving all files; possibility to work on a long time project; editing NDSPUB control file to finalize PS/PDF output
- Administrating tools

Submitting and distributing ENSDF codes: NDS has a long experience in distributing data, codes and integrated systems on CD/DVD ROM's and via Web downloading. Some of these products are rather complex and include software (internal programs written in Java, Fortran, C and external), large databases and usually can work on most popular platforms (Windows, Linux, Mac). The policy of NDS in distribution of such systems is described in [1]. Examples include: EXFOR-CINDA retrieval systems, ENDVER/GUI package, Portable Empire.

A set of rules regulating submission of new codes to distributing centres (NDS and/or NNDC) was presented and proposed for discussion. These rules include the provision of the source and make files by authors, set of automatized examples (scripts, executables, standard input and output files), etc. An example of such a system of files for the Fortran code RadD was given to participants and is included in Appendix A.

Discussion: Requirement to supply source codes can have exemptions (if it is in conflict with the policy of author's organization); such cases can be regulated by special agreement with the author.

Light EXFOR Editor as possible technology for a new web based ENSDF Editor: A pilot project "Light EXFOR Editor" presenting EXFOR file as an interactive tree data structure with possibility of editing was demonstrated on-line for the meeting participants. This editor is under development, but ideas and technology can probably be used for the development of a new, web based, ENSDF Editor. The time and effort that would be required for full implementation of this approach should be estimated before any final decision is taken.

Reference

[2.8.1]   CD-ROMs Produced and Distributed by the IAEA Nuclear Data Section: Standard Procedures and Inputs, by V. Zerkin, INDC(SEC)-0108, Vienna, November 2007.

3. TECHNICAL DISCUSSION

3.1. PROGRESS REVIEW

One of the outstanding issues regarding the development and improvement of the ENSDF Analysis codes that was discussed at the meeting is the treatment of asymmetric uncertainties. To date, none of the existing analysis codes is programmed to handle asymmetric errors. This is a serious deficit in the analysis codes which can impact on the quality of the evaluation.

Participants discussed several methods that are used to calculate asymmetric uncertainties, however it was agreed that further work is needed to explore the available methods in detail and perform extensive testing. Once the method has been agreed upon, the procedure for treating them in all the ENSDF analysis codes can be determined and adopted by the NSDD network.

Action on Kibédi, Birch: explore methods for treating asymmetric uncertainties and propose procedure for treating them.

The treatment of systematic uncertainties was also discussed and it was suggested that evaluators from NSDD and DDEP should consult experts for recommendations.

The discussions relating to the individual codes are summarized in the following sections.

3.1.1. VISUAL AVERAGING LIBRARY

The Visual Averaging Library has been re-written in JAVA by M. Birch so that it is portable on all platforms. Certain improvements were discussed such as including a plotting routine.

In this respect it was suggested that implementing well-known and freely distributed graphics packages would be an efficient way of doing the job and would save the developer time. It was also suggested that adding the outliers that were not included in the averaging procedure would be helpful to the user.

Action on Birch: include Barlow's prescription for treating asymmetric uncertainties based on defining a likelihood function in V. AveLib and provide working version for distribution.

Action on Birch, B. Singh, Kibédi: prepare a manual describing the different methods including recommendations for different methods in different situations.

It was also suggested that an effort should be made to replace the two averaging codes, Visual Averaging Library and AveTools by a single code that would include all approved methods for distribution to the network evaluators.

Action on Kibédi: look into the two averaging codes and advise J. Tuli on which one should be maintained and distributed to the network evaluators. Further action will be taken accordingly.

3.1.2. JAVA NDS

The JAVA NDS code, initially developed by McMaster Univ. for the purpose of producing publishable PDF output from ENSDF, has recently been revised by MSU in collaboration with McMaster Univ. The improved output of the code will be distributed to interested

meeting participants and other NSDD evaluators for comments and feedback. After the suggested modifications have been implemented, the beta version of the code will be distributed to the network by the end of November.

Action on Tuli: set up a specialists meeting to review the beta version of JAVA NDS and decide upon final output form.

JAVA NDS can also be used for producing a web display of ENSDF. The form that could be used (PDF or html) will depend on the decision of those responsible for maintaining the ENSDF web display. If the decision is to use this code for html then further work will be required.

3.1.3. RULER

Two codes are foreseen with similar operating functions, PYRULER and TRULER, the former being a stand-alone version only.

PYRULER: a new interactive reduced transition probability code has been developed in PYTHON. The code includes the PYTHON 'uncertainties' package. The code will also treat limits and asymmetric uncertainties for quantities such as half-lives ($T_{1/2}$), branching ratios (BR), intensities and mixing ratios (MR) using a MC approach.

It was suggested that guidelines on the environment specifics need to be distributed along with the code.

TRULER: will be based on the newly developed NS_lib library and will work on an ENSDF file. The code will treat asymmetric uncertainties using a procedure that will be recommended for all NSDD codes.

A beta version of the code will be available for testing by June 2016.

3.1.4. JGAMUT

A code for calculating gamma-ray energies and intensities from multiple data sets was developed following an approach similar to the previous GAMUT code [3.1.1] and submitted to the meeting participants for testing prior to this meeting.

The new code, written in JAVA, is currently in its beta stage. Feedback received prior to the meeting and during this meeting (see Sect. 2.2 and Annex 3) will be implemented. The improved beta version will be circulated to the NSDD network by the end of November 2015. The feedback from NSDD evaluators will be implemented in the code and a stable version will be distributed by May 2016.

Further development including a visual interface (GUI) for the intermediate file and possible addition of levels without gammas is also desirable.

Reference

[3.1.1]   Firestone, R. B., (1991). GAMUT: A Computer Code for gamma-ray Energy and Intensity Analysis. - Report Number: LBL-26024.

3.1.5. BRICCEMIS

Significant progress has been made in the development of the new code that calculates atomic radiation spectra using a Monte Carlo calculation of atomic vacancies and propagation. The atomic radiation data calculated by this program will be incorporated in the ENSDF file in data continuation record format. The exact format is yet to be determined.

Currently BrIccEmis does not calculate beta spectra. In the future it will read the beta spectra produced from the Beta Shape Analytic code (see 3.1.7) developed by X. Mougeot.

Further progress and developments shall be presented at the next meeting on ENSDF Analysis codes in 2017.

3.1.6. LOGFT

The existing code needs to be modified to provide warning messages in cases where the input data is unphysical. The recommendation was that this request for modification should be submitted to NNDC through the GFORGE environment at NNDC.

Other improvements that are considered necessary are:

1. Asymmetric uncertainties are not allowed in the data fields but can only be inserted in the continuation record. This means that in the PDF output or web display, the asymmetric uncertainties will appear in the Comments section whereas they should appear in the data field.
2. Higher order transitions e.g. 3rd Forbidden Unique (FU), which are important for certain nuclides such as 40K, are not treated in the current code. Evaluators use the existing data on allowed, 1st FU, and 2nd FU, to extrapolate to 3rd FU. This procedure, although crude, is in agreement with more reliable model calculations (Mougeot).
3. Very low-energy beta-transitions cannot be handled correctly.

The new beta shape code (see sect. 3.1.6) developed by Mougeot can treat both (2) and (3) for $\beta^{\pm}$ transitions (not EC) more precisely. Until this new code is distributed, it was suggested that Mougeot provides results for higher-order FU and low-energy transitions to the NSDD evaluators upon request. Work for including EC in the beta shape code is in progress.

3.1.7. BETA SHAPE

The code bsan that calculates the beta spectra shape factors for $\beta^{\pm}$ transitions using analytical expressions for allowed and FU, and the ξ–approximation for Forbidden Non-Unique (FNU) transitions. A code that will calculate EC transitions is also under development. It was recommended that apart from the spectra, these codes should also provide the logft values obtained from integrating over the beta shape function and propagate uncertainties from the input parameters.

An executable version of the bsan code is expected to be distributed to NSDD evaluators after it has been completed and tested.

3.1.8. CHECKING CODES

FMTCHK: It was agreed that updating the code to include all the new quantities that have been entered into ENSDF since 2007 is of top priority. Requests and recommendations should be submitted on GFORGE at NNDC. [**Sec. note**: subsequent to the meeting FMTCHK has been modified to substantially eliminate excessive warning messages and reduce clutter in output error file].

PANDORA: additional physics and consistency checks need to be included in the existing code and evaluators are encouraged to submit requests or suggestions via GFORGE at NNDC. Evaluators who do not have an account on GFORGE can request one from NNDC (arcilla@bnl.gov).

Evaluators interested in helping with these codes should contact J. Tuli.

Efforts should also be made to collaborate with the Petersburg Nuclear Physics Institute (PNPI) group which has developed several checking codes that perform specific checks and provide detailed error reports.

Action on PNPI group: Provide manual describing the functions of the codes and the meaning of the error messages.

Action on Zerkin, Rodionov: upload all the PNPI checking codes on Myensdf Web tools and organize them in such a way that they can be run separately or as a chain of codes.

Action on NDS-IAEA: enhance collaboration with PNPI group to facilitate the dissemination of their codes.

3.1.9. ALPHAD

A new code RadD was developed to deduce the radius parameter r_0 for odd-A and odd-odd nuclides using the Alkovali tables [2.6.3]. This code has now been appended to the ALPHAD code. Apart from further improvements that were suggested in Sect. 2.4 (see also Annex 3), the next major task is now to update the Alkovali r_0 tables for even-even nuclides. This work is in progress. The table can be made available by February 2016.

The ALPHAD+RadD code including the new table will be tested and then distributed to NSDD evaluators for additional comments by May 2016.

3.1.10. MODULAR STRUCTURE LIBRARY (ENSDF FORTRAN API)

NS_lib-subroutine library: The subroutine that reads complete data sets into memory, converts and verifies the numerical values and uncertainties of all fields from primary and continuation records, and performs format and syntax checking, has been developed with the aim of being shared by all ENSDF analysis codes that will in turn be written in modular form.

The library subroutine will be accompanied by other high-level subroutines that will perform common tasks for all the codes, such as calculating Internal Conversion Coefficients (ICC) & total intensities, level scheme normalization, and uncertainty propagation.

To achieve the above task an updated ENSDF Manual is required.

This modular structure is planned to be implemented to BrICC, BrICCemis, TRULER, and the new GABs.

It is expected that eventually all ENSDF analysis codes will be re-written in this modular structure with a common shared NS_lib subroutine.

In the future, similar API should be developed for other programming languages such as JAVA, C/C++.

3.1.11. EVALUATION TOOLKIT

Three options were mentioned for developing and disseminating an Evaluation Toolkit:

OPTION A. Starting from the existing EVP Editor developed by A. Sonzogni (NNDC-BNL), upgrade and further develop the application, and make it available on the online codes dissemination web pages.

OPTION B. Starting from the existing Evaluation Toolbox, developed by the PNPI group, re-write the software in a modern programming language such as JAVA, in collaboration with PNPI. Also include further development of application.

OPTION C. Work on extending the tree-level structured web-based editor applied to the EXFOR database to ENSDF and link with Myensdf Web tools to provide a compact toolbox (V. Zerkin). Liaise with developers of JAVA NDS code for sharing common JAVA classes and with expert NSDD evaluators to implement the ENSDF format.

Participants acknowledged the importance of developing an evaluation application that a) would allow the evaluator to produce an ENSDF file through a user-friendly and format-independent interface, b) would integrate all the analysis and utility codes relieving the evaluator of having to download, install, compile and debug each code separately, and c) would serve as a viewer of the ENSDF file including graphics.

For all the above reasons, meeting participants support the new proposal by V. Zerkin and will collaborate with him to accomplish this task. At the same time they also encourage continuation of development of the other two options, namely the EVP editor and the PNPI group editor.

3.2. REQUIREMENTS FOR CODE DEVELOPMENT

3.2.1. DOCUMENTATION

All new and existing codes should be accompanied by detailed documentation covering the physics models, the methodology, and treatment of uncertainties.

The code manual should also give guidance on the interpretation of the results and error messages.

Test cases should be provided with every code with appropriate documentation.

3.2.2. REQUIREMENTS FOR CODE DEVELOPERS

The following requirements for code developers intending to submit new codes within this IAEA project were discussed and adopted at the meeting:

1. Recommended languages: F90, Java, C, C++, Python
2. I/O Library for every programming language (with separated input, calculations, output in order to re-use I/O in different programs)
3. Executable (-static) for 3 platforms: Windows, Linux, Mac-OSX; Portable systems can be considered)
4. File readme.txt explaining how to run the code (short)
5. Prepared tests, e.g.: run1.sh, run1.bat, run1.tti , run1.tto-0 , run1.err-0 prepared for quick start and testing in local user's environment, where run.tto-0 contains original output provided by author
6. Command-line regime (relevant for programs having GUI)
7. Providing source and make files to a distributing centre (and/or for public) with possibility to rebuild executable in other environment in the future
8. Public re-distribution of source can be regulated by special agreement between author and distributing centre
9. Standard data files should be stored in a single directory and programs should access it using an environment variable; default value of this variable should be the current directory path

4. ENSDF POLICIES AND FORMATS

It was agreed that the ENSDF evaluation policies and formats related to the functioning of these codes should be updated and made available to the code developers and the members of the NSDD network at large. It was recommended that all the new codes should comply with the ENSDF policies.

An electronic Format Manual has been created for NS_lib subroutine by T. Kibédi based on the ENSDF Manual (BNL-NCS-51655-01/02-Rev). It was suggested that this manual is made available on GFORGE to facilitate the submission of requests for improvement and further enhancement. As a first step in this direction, T. Kibédi and M. Verpelli volunteered to provide a complete list of currently used quantities on continuation record in ENSDF for consideration in the revision of the manual.

The complete and updated document will become available on the NNDC web page.

4.1. VALIDATION

All codes should be rigorously tested by the code developers and experienced evaluators before the final distribution of a stable version. This effort should be coordinated by the developers themselves. The validation procedure should involve the following:

-testing the codes run properly on all platforms

-test for spurious results and bugs

-test for the correctness of the results

In this respect, test cases could be defined and provided by the program developers for all operations and branches of the codes on all platforms. All evaluators participating in the validation should report their findings directly to the code developer/coordinator.

The list of coordinators and candidate evaluators who will be responsible for validating these codes prior to their dissemination to the whole network is given in Table 2.

4.2. DISSEMINATION OF CODES

Developers are required to provide stable versions of their validated codes to NNDC/BNL and IAEA-NDS either as executables for all three operating systems, namely, Windows, Linux and MAC OS, or as source codes. In the latter case, they should also provide suitable Makefiles that would allow the user to compile the source codes on the desired platform. An example of the Makefile prepared by V. Zerkin is included in Appendix A.

5. CONCLUSIONS

The Data Development Project initiated by the NDS IAEA to address the problems of updating and maintaining the Analysis and Utility Codes used by the evaluators of the network of Nuclear Structure and Decay Data in mass chain evaluations (ENSDF) held its 2nd Technical Meeting at IAEA Headquarters in Vienna, from 5 to 8 October 2015.

Participants of the meeting reviewed the progress in the development of new codes and improvement of the existing ones, re-assessed the emerging needs, revised the priority list of codes that need to be modified and/or re-written accordingly, and produced a list of actions (see Tables 1 and 3). Validation groups were formed to test the new codes under development in coordination with the code developer (see Table 2).

Progress reports will be made at the upcoming USNDP and NSDD meetings, however, a comprehensive review of the project and update of priorities will be the subject of a follow-up meeting to be held in Vienna in 2017.

6. LIST OF ACTIONS

Table 1. Revised tasks.

CODES	PRIORITY	WORK	RESPONSIBLE	TIMELINE
WEBTREND/ENSDAT (EMPHASIS ON WEB RETRIEVAL)	1	ACCURATELY REFLECT THE CONTENTS OF THE ENSDF/XUNDL DATABASES	NNDC	IN PROGRESS
JAVA NDS	1	FURTHER DEVELOPMENT AND TESTING	J. CHEN, B.SINGH	BETA-VERSION END OF NOVEMBER 2015
TRULER **PYRULER**	1	DEVELOPMENT DEVELOPMENT AND TESTING	T. KIBÉDI, F. KONDEV M. BIRCH	BETA VERSION BY JUNE 2016
JGAMUT	1	IMPROVEMENT AND TESTING	M. BIRCH, B. SINGH	BETA VERSION BY END OF NOVEMBER 2015
EVALUATION TOOLKIT (EDITOR+CODES)	2	EXPLORE DIFFERENT OPTIONS	COORDINATED BY NDS IAEA (SONZOGNI, PNPI, ZERKIN)	IN PROGRESS-OPTION C TO START END OF SUMMER 2016
NS_LIB	1	DEVELOPMENT AND TESTING	KIBÉDI	NEXT CODES MEETING
BRICCEMIS	2	DEVELOPMENT	T. KIBÉDI	IN PROGRESS REPORT AT NEXT CODES MEETING
BETA SHAPE ANALYTIC	2	BETA +- TRANSITION: IMPROVEMENT + TESTING FOR EC: DEVELOPMENT	X. MOUGEOT	JANUARY 2016 NEXT CODES MEETING
CHECKING CODES (FMTCHK)	1	ENHANCE FORMAT CHECKING AND PHYSICS CHECKING CAPABILITIES	NNDC INVOLVE PNPI GROUP	CONTINUOUS
PANDORA	2	ENHANCE CODE	J. TULI-NSDD NETWORK	CONTINUOUS
NEW R0 INTERPOLATION CODE	1	INCORPORATION IN ALPHAD	S. SINGH, B.SINGH	IN PROGRESS FEBRUARY 2016
NEW R0 TABLES		UPDATE R0 TABLES FOR NEW Q-VALUES, BRANCHINGS AND NUCLIDES	B. SINGH, S. SINGH	
VISUAL AVERAGING LIBRARY	1	INCLUDE BARLOW METHOD AND PLOTTING	M. BIRCH, B. SINGH	END OF NOVEMBER 2016
LOGFT	2	WARNING MESSAGES FOR UNPHYSICAL INPUT DATA AND ASSIGNMENT OF UNCERTAINTIES	NNDC	PENDING
ONLINE WEBTOOL	2	MAKE ALL PNPI CHECKING CODES AVAILABLE	V. ZERKIN	MID-2016

Table 2. Validation groups.

CODES	DEVELOPER	VALIDATION
JAVA NDS	CHEN	SINGH,VERPELLI
TRULER	KIBÉDI	BROWNE, KONDEV, MCCUTCHAN, SINGH
JGAMUT	BIRCH	CHEN, KIBÉDI, KONDEV, MCCUTCHAN, SINGH, KELLETT
BRICCEMIS	KIBÉDI	BROWNE, KONDEV, MCCUTCHAN, KELLETT
BETA SHAPE ANALYTIC	MOUGEOT	KIBÉDI,KONDEV
ALPHAD	SINGH/SINGH	BROWNE, KONDEV, SINGH

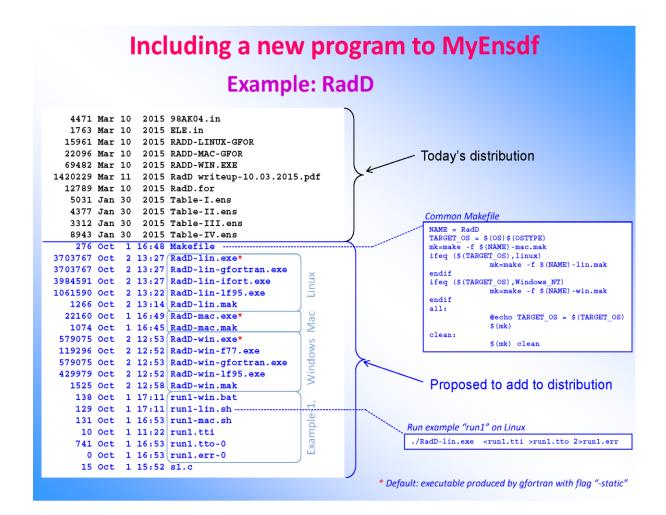**Table 3. Summary List of Actions.**

#	Action	Person Responsible
1	Explore methods for treating asymmetric uncertainties and propose procedure for treating them	Kibédi, Birch
2	Include Barlow's prescription for treating asymmetric uncertainties based on defining a likelihood function in V. AveLib and provide working version for distribution	Birch
3	Prepare a manual describing the different methods including recommendations for different methods in different situations.	Kibédi, Birch, Singh
4	Look into the two averaging codes and advise J. Tuli on which one should be maintained and distributed to the network evaluators.	Kibédi
5	Set up a specialists meeting to review the beta version of JAVA NDS and decide upon final output form.	Tuli
6	Provide manual describing the functions of the codes and the meaning of the error messages.	PNPI group
7	Upload all the PNPI checking codes on the Myensdf Webtool and organize them in such a way that they can be run separately and as a chain of codes.	Zerkin, Rodionov
8	Enhance collaboration with PNPI group to facilitate the dissemination of their codes.	IAEA NDS

REQUIREMENTS FOR SUBMITTING A NEW CODE

To establish a common procedure for testing new codes on all widely used OS and disseminating them for all platforms, the following requirements for submitting a new code to the IAEA NDS were adopted at this meeting:

Codes should be submitted either as executables for all three platforms (Windows, Linux, MAC), in which case the compilation should be 'static', or as source codes, in which case the makefiles for compilation should also be provided for Windows, Linux (using standard free gfortran compiler) and MAC OS. In addition, script files (batch, shell scripts etc) should be provided for a standard run using standard input and output files, so that the tester/user knows what to input and what to expect as output.

An example was given for the new code RadD as shown below (see V. Zerkin in Annex 3):

Appendix A

An example of a makefile for Linux is also given:

```
NAME = RadD
platform=-lin
O = o
F = for
C = c
NAMEEXE0= $(NAME)$(platform).exe
NAMEMAK = $(NAME)$(platform).mak
NAMEEXE = $(NAMEEXE0)

SRC1 = RadD.$(F) s1.c
SRC2 =

SRC  = $(SRC1) $(SRC2)
OBJX = $(SRC:.$(C)=.$(O))
OBJS = $(OBJX:.$(F)=.$(O))

CC     = gcc
CFLAGS = -c

FC = gfortran
#FC = ifort
#FC = lf95
FFLAGS = -c

NAMEEXE = $(NAME)$(platform)-$(FC).exe

LINK =$(FC)
LFLAGS = -o $(NAMEEXE) -static

#Flags based on compiler setting
ifeq ($(FC),gfortran)
    #----GNU FORTRAN compiler
    FFLAGS = -c
endif
ifeq ($(FC),ifort)
    #----INTEL f95 compiler
    FFLAGS = -c -m64
endif
ifeq ($(FC),lf95)
    #----Lahey/Fujitsu f95 compiler
    FFLAGS = -c -m32
    LFLAGS = -o $(NAMEEXE) -static
    CFLAGS = -c -m32
endif

$(NAMEEXE) : $(NAMEMAK) $(OBJS)
    @echo -----Link to produce $(NAMEEXE)
    $(LINK) $(OBJS) $(LFLAGS)
    @echo -----Link done
    @echo -----Copy $(NAMEEXE) to $(NAMEEXE0)
    @cp $(NAMEEXE) $(NAMEEXE0)
    @ls -la $(NAMEEXE)

%.$(O) : %.$(F)
    @echo -----Compile $<  by $(FC)
```

Appendix A

```
     $(FC) $(FFLAGS) $<

%.$(O) : %.$(C)
     @echo -----Compile $< by $(CC)
     $(CC) $(CFLAGS) $<

clean :
     rm -f $(OBJS)
     rm -f *.mod
     rm -f *.map

cleanall :
     rm -f $(NAMEEXE)
     rm -f $(OBJS)
     rm -f *.mod
     rm -f *.map
```

```
     $(FC) $(FFLAGS) $<

%.$(O) : %.$(C)
     @echo -----Compile $< by $(CC)
     $(CC) $(CFLAGS) $<
```

Appendix A

2nd Technical Meeting on
Improvement of Codes for Nuclear Structure and Decay Data Evaluations

IAEA Headquarters, Vienna, Austria
5 – 8 October 2015
Meeting Room M0E100

ADOPTED AGENDA

Monday, 5 October

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

09:30 – 10:00   **Opening Session**
Welcoming address
Administrative matters
Election of Chairman and Rapporteur
Adoption of the Agenda

10:00 – 12:30   **Presentations by participants**

1) PYRULER, (Kondev)
2) JGAMUT and V.AveLib, (Birch)
3) JAVA NDS, (B. Singh)
4) Beta-spectra, (Mougeot)
5) NS_Lib - subroutine library (Kibédi)
6) RaDd-ALPHAD, (S. Singh)
7) GFORGE at NNDC (Tuli)
8) RADLIST, LOGFT, (Rodionov)
9) Feedback on JAVA NDS, (Verpelli)
10) Progress in MyEnsdf web tools for ENSDF evaluators, (Zerkin)

12:30 – 14:00   *LUNCH*

14:00 – 17:30   **Presentations by participants (cont'd)**

Coffee break as needed

Tuesday, 6 October

09:00 – 12:30   **Presentations by participants (cont'd)**

Coffee break as needed

12:30 – 14:00   *LUNCH*

14:00 – 17:30   **Round Table Discussion**

Progress review
Validation process: how and who
Dissemination/software package requirements
New priorities/review of assignment list
Other

Coffee break as needed

19:00 Dinner at local restaurant

Wednesday, 7 October

09:00 – 12:30   **Round Table Discussion (cont'd)**

Coffee break as needed

12:30 – 14:00   *LUNCH*

14:00 – 17:30   **Round Table Discussion (cont'd)**

Coffee break as needed

Thursday, 8 October

09:00 – 12:30   **Drafting of the Summary Report**

Coffee break as needed

12:30 – 14:00   *LUNCH*

14:00 – 16:00   **Drafting of the Summary Report (cont'd)**

16:00   **Closing of the meeting**

2nd Technical Meeting on

Improvement of Analysis Codes for Nuclear Structure and Decay Data Evaluations

IAEA Headquarters, Vienna, Austria
5 – 8 October 2015

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2nd Technical Meeting on
Improvement of Codes for Nuclear Structure and Decay Data Evaluations

IAEA Headquarters, Vienna, Austria
5 – 8 October 2015

Links to Presentations given at the meeting:

#	Author	Title	Link
1	F. Kondev	RULER - stand-alone version	PDF
2	M. Birch	JGAMUT: ENSDF Adopted Levels, Gammas Assistant Code	PDF
3	B. Singh	JAVA-NDS computer code	PDF
4	B. Singh	Nuclear Data Sheets for A=40*	PDF
5	X. Mougeot	Improvement of analytical calculations of beta spectra	PDF
6	T. Kibedi	NS_Lib - subroutine library	PDF
7	S. Singh	Revised ALPHAD (ALPHAD+RadD)	PDF
8	J. Tuli	Development of Codes on GFORGE	PDF
9	A. Rodionov	ENSDF: remarks concerning the politics and the Manual	PDF
10	A. Rodionov	Programs RADLIST, LOGFT and PANDORA, critical analysis	PDF
11	V. Zerkin	Progress in MyEnsdf (web tools for ENSDF evaluators)	PDF

Annex 3

Annex 4

Group Photo

Annex 4