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INDC International Nuclear Data Committee

Summary Report of Technical Meeting

Improvement of Analysis Codes for Nuclear Structure and Decay Data Evaluations

IAEA Headquarters, Vienna, Austria

10 - 13 June 2014

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September 2014

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Abstract

A summary is given of a Technical Meeting assembled to assess the current status of the 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 codes and discussed emerging needs for improved physics models, error treatment, physics and format checking and modernisation of the programming tools including the use of online webtools and a user-friendly evaluation toolkit to facilitate the evaluators' work. The meeting produced a list of priorities of the codes and the modifications that need to be made and assigned tasks to individual participants. Details of the discussions and the proposed work plan are presented in this summary report.

September 2014

Table of Contents

1. INTRODUCTION

The Nuclear Structure and Decay Data Network (NSDD) consists of evaluation groups and data centres in several countries and has the objective of providing up-to-date nuclear structure and decay data for all known nuclides by evaluating existing experimental data. The recommended "best values" for the various nuclear structure and decay data are included in the Evaluated Nuclear Structure Data File (ENSDF) and published in the journals *Nuclear Physics A* and *Nuclear Data Sheets*. This international evaluation collaboration is coordinated by the IAEA Nuclear Data Section (IAEA NDS).

The National Nuclear Data Centre (NNDC) maintains and distributes various programs in support of the NSDD network. These programs generally use input files in ENSDF format.

The ENSDF Analysis and Utility codes are essential tools for analysing the various types of experimental data available in the literature, including level-schemes, spin-parities, level half-lives, transition energies, intensities, multipolarities, etc. By combining the nuclear data from different decay channels and reactions the adopted properties of a given nucleus are collated into the so called Adopted data set. The accuracy, consistency and reliability of the recommended values in the ENSDF database, depends largely on the analysis and utility codes. It is therefore of vital importance that these codes are kept in good condition and are properly maintained. In practice, maintaining these codes implies that they are continuously checked for bugs, kept up-to-date with developments in physics models, statistical methods and error analysis, and evaluation policies in general.

Most of the codes are written in ANSI standard FORTRAN 77 and have been made compatible with FORTRAN 95. They are accompanied by "read me" files that give a basic description of the programs, input and output files, special options, terminal dialog, compilation and loading instructions, revision history, and references to additional documentation if available. They are also accompanied by executables for operating systems such as Windows (including source files program), Linux or Unix (including source files), and MacOS.

To make sure that these codes are properly maintained in the future, and remain fully operational for all Operating Systems, there is a need to review their status, update the physics models, analysis and checking capabilities where necessary, and in some cases re-write them using more modern programming languages such as FORTRAN 90/95, Java, and C++.

The NSDD network has expressed its concern about the status and future of the ENSDF analysis and utility codes at the recent Technical Meetings organized by the IAEA NDS. In response to these concerns, IAEA NDS has taken action by initiating an international project that aims to address all the outstanding issues related to the ENSDF codes. A Technical Meeting was held from 10 to 13 June 2014, at the IAEA Headquarters in Vienna, with the purpose of

- producing a priority list of codes that need to be addressed,
- identifying the type of modifications and how to implement them in accordance with the General Policies
- outlining general requirements of any ENSDF code (programming language, structure, documentation)
- identifying all possible means to make these codes user-friendly and efficient to all evaluators especially the new generation web tools, evaluation toolkit etc)
- assigning tasks and responsibilities to participants in this project

On the first day of the meeting, participants from Canada, Australia, France and USA (see Appendix 2 for Participant's List) were welcomed to the IAEA by the Head of the Data Development Unit of the Nuclear Data Section, Roberto Capote Noy, who acknowledged the importance of the new project for the work carried out by the NSDD network. The Scientific Secretary, Paraskevi Dimitriou, 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 Appendix 1) and the meeting began with participant's presentations (see Appendix 4 for links to the presentations).

2. PRESENTATIONS BY PARTICIPANTS

2.1 Introduction to ENSDF-related Computer Programs (Jagdish K. Tuli, Brookhaven National Laboratory, USA)

The computer programs fall in the following categories:

Utility Programs: Programs needed for the maintenance of the ENSDF database. In this category the main program is FMTCHK. This program is run on all ENSDF files multiple times before the datasets are added on to ENSDF. The program needs to be kept up-to-date maintain integrity of ENSDF.

Analysis Programs: These are programs used in evaluation of data. Various programs, namely, BRICC, LOGFT, RULER, RADLIST, GTOL, PANDORA were briefly described and their current status discussed.

Publication Programs: NDSPUB, and its limited version ENSDAT, were described.

Dissemination Programs: Various dissemination techniques and formats were mentioned and their needs were described.
Current status and priority to update of the various codes was suggested.

2.2 Outstanding issues of ENSDF Codes (Filip G. Kondev, Argonne National Laboratory, USA)

The presentation made by the ANL staff emphasized on the opportunity to revitalize the old-legacy ENSDF codes and to improve their physics capabilities, which could have a significant impact on the ENSDF quality and productivity.

The present situation with the maintenance and update of the ENSDF analysis codes, and the corresponding auxiliary input files, is not satisfactory. Most of the programs have not been updates since 2007, they do not have proper manuals that describe the assumptions made and how the uncertainties are treated, thus making their future upgrade rather complex and difficult.

Requirements for the newly developed codes were outlined, including the need the new programs a) to run on the three major OS – Windows, Linux and Mac OSX; b) to be rigorously tested before officially distributed, including creation of test samples; c) to have a detailed manual, including installation instructions, physics assumptions and computational structure, as well as how the uncertainties are treated, similarly to the manuals available for BrICC & RADLIST; d) to be disseminated from several (independent) repositories, e.g. IAEA, NNDC, and others; e) the effort to be coordinated, so the duplication of effort is avoided; and e) the effort to be prioritized, so that we start with the most urgent needs and continue with the rest as time permits.

An example was presented with the RULER program that fails to calculate correctly the gamma-ray transition probabilities. This program was given highest priority and the ANL and ANU participants proposed to develop a new code that would be distributed to the NSDD network following the above guidance.

Another code that will be developed at ANL, in collaboration with ANU, would assist in decay data evaluations, eventually replacing a suite of presently operating programs.

At the end of the presentation, a newly developed at ANL tool, named xls2ens, was presented. It allows a creation of an ENSDF data set from a pdf-formatted file via an intermediate xls formatted file.

2.3 *Recommended Gamma-ray Energies and Intensities from Multiple Datasets -Revival of GAMUT-type computer code (Balraj Singh, McMaster University, Canada)*

ENSDF evaluations produce recommended values of gamma-ray intensities and energies for use in a variety of fields, including: nuclear reactors, nuclear medicine, nuclear astrophysics and nuclear structure theory. This process involves combining experimental data from decays and reactions into a single set of "*adopted values*".

Currently, most ENSDF evaluators seem to use a "gamma-by-gamma" approach in which they manually take the weighted average of the set of measurements that have been made for each observed gamma-ray. This is done for both energy and intensity measurements. Finally, the evaluators run GTOL on the adopted energies and intensities. The disadvantage

of this approach is that it is labour intensive, but also that it considers gamma-rays individually so there is no standardized way of identifying and correcting inconsistencies in efficiency and energy calibrations between experiments. These problems could be addressed through a gamma-ray energy and intensity evaluation code.

GAMUT Code

The GAMUT code was written circa 1982 by R. B. Firestone at Lawrence Berkeley National Laboratory. This code helped to automate the evaluation process and had a number of other features including: outlier detection, uncertainty adjustment for discrepant measurements, correction factors for energy calibration using level scheme fitting (similar to GTOL), and correction for differences in efficiency calibrations by fitting parameters obeying linear relations between the intensity scales.

GAMUT-Type Code Proposal

We propose that a new GAMUT-type code should be written for the purpose of gamma-ray energy and intensity evaluations. This code will take ENSDF-format input data sets, process them into an intermediate file which can be edited by the evaluator, then use the intermediate file to run the proposed computer code, and generate final output. The output should consist of an ENSDF-formatted file containing the adopted levels and gammas and a report file with details about the calculation such as chi-square analysis, outlier flags and other warnings. We propose the method to be used for determining recommended gamma-ray energies to be as follows: determine energy calibration shifts (by level-scheme fitting, and with reference to the most reliable dataset, or some other statistical approach), apply the shifts to the data sets then take a gamma-by-gamma weighted average, then finally run GTOL on the adopted gamma-ray energies. We propose the gamma-ray intensity evaluation method should be the same as in the original GAMUT. This code would be advantageous to the evaluator community by partially automating the evaluation process, providing consistency in evaluations between different evaluators and accounting for systematic differences between data sets. We propose this code be written in Java since it will then be platform independent and easily maintained in the future. The writing of the proposed computer code could start in September 2014.

2.4 *BrIcc and related codes to evaluate conversion coefficients and atomic radiations in nuclear decay (Tibor Kibédi, Australian National University, Australia)*

Internal conversion coefficients provide important information about the atomic nucleus. Through comparison of experimental values with corresponding theoretical ones, multipolarities and mixing ratios of nuclear transitions are determined. As well as nuclear structure research, knowledge of accurate coefficients is needed, for example, in the determination of total transition rates (required for the normalization of decay schemes), Mössbauer spectroscopy (CEMS), nuclear reaction calculations, or decay heat calculations of spent nuclear reactor fuel cells.

The most accurate theoretical conversion coefficient table is based the relativistic Dirac-Fock method. To make the new theoretical values accessible for a very broad user community a new internal conversion coefficient database called BrIcc has been developed in an international ANU - NNDC - Petersburg - ORNL collaboration. Over the years a range of

programs has been developed to help ENSDF evaluators and the scientific community. All programs are written in FORTRAN 90 and distributed for Windows, Linux and MacOS operating systems.

BrIcc (v2.3 7-Aug-2013)
The console program can be used interactively to obtain conversion coefficients for a given atomic number, transition energy, multipolarity and electron shell. The internal conversion coefficient table is based on the so called "frozen orbital" approximation, which is in excellent agreement with a wide range of high precision experimental conversion coefficients. BrIcc also can be used as an evaluation tool to create and insert special records into ENSDF files. The program can be obtained from the NNDC website: http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/. A comprehensive program manual is also available, which describes BrIcc and BrIccS.

BrIccS (v2.3 2-Sep-2013)
A silent version of the BrIcc code, developed for applications, where the detailed knowledge of the conversion coefficients is required, including multipolarities, mixed transitions, etc. BrIccS shares procedures and subroutines with BrIcc. BrIccS can be obtained from the ANU web site: http://bricc.anu.edu.au/bricc-obtaining.php

BrIccMixing (v2.3 17-Jan-2014)
This program can be used to determine multipole mixing ratio from data set(s) compiled from conversion coefficients, conversion electron intensities or ratios of these. The input file also can contain mixing ratios determined from gamma-ray measurements. A short manual and sample input files together with the code can be obtained from the NNDC: http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/

BrIccEmis (under development)
A new program is being developed in an ANU-ANL (F. Kondev) collaboration to evaluate the complete spectrum of the atomic radiations, including X-rays and Auger electrons from radioactive decay. Initial vacancies can be created in electron capture decay and internal conversion processes. The subsequent atomic relaxation process is treated stochastically.

General comments
The above codes share a range of FORTRAN routines to read, parse and verify ENSDF files, evaluate conversion coefficients and treat uncertainties according to the procedures described in the BrIcc manual. Extensive use was made of the derived types, or structures, to store a collection of named components (value, uncertainty, ASCII and numerical value, error flags, etc.) related to a given physical quantity. This coding approach is very powerful in developing codes and creating portable subroutines.

Future directions
Two new data tables have been developed as an extension to the BrIcc data tables. A detailed conversion coefficient table was calculated for super heavy elements. A second table on the E0 electronic factors is being developed. These tables will be accessible through the new version of BrIcc. The first test version is expected to be released in 2015.

2.4 *Calculation of beta spectra – The most common assumptions and how to go beyond (Xavier Mougeot, Laboratoire National Henri Becquerel (LNE-LNHB), France)*

The Fundamental Data Cell within the National Laboratory Henri Becquerel (LNHB) is in charge of atomic and nuclear data evaluations. Our users have asked for many years a precise knowledge of beta spectra, coupled with well-established uncertainties. For that purpose, we have led off a study of these spectra, both experimentally and theoretically. Two experimental techniques are available at LNHB: metallic magnetic calorimeter for low energies, and silicon detectors for medium energies. This presentation is focused on the calculation of beta decay processes.

First, the basics of beta decays and the most common assumptions used to calculate spectra shapes are presented. Intrinsically, the nuclear structure is coupled to the leptons dynamic, which makes the calculations highly difficult. Thus, all the assumptions are chosen in order to simplify as much as possible the calculation: neutrino massless, nucleus described as a point charge, recoil energy of the nucleus neglected. An analytical code, named BetaShape, has been developed according to these assumptions dealing specifically with allowed and forbidden unique transitions, calculating the non-unique ones according to the ξ approximation, and including rough analytical corrections for screening and finite nuclear size effects, and for the radiative corrections.

Compiling a small, but almost comprehensive, database of 130 experimental shape factors available in the literature, very few measurements below 50 keV and very few transitions of high forbidding order were found. A systematic comparison with the calculations leads to the following results: the usual $\lambda_k = 1$ assumption to calculate forbidden unique spectra results generally in poor agreement; allowed and forbidden unique spectra are generally reproduced well; ξ approximation is correct only for about 50% of the first forbidden non-unique transitions, and wrong for all other cases. These results are illustrated with the beta spectra from ^{90}Sr, ^{172}Tm, ^{210}Bi and ^{36}Cl decays. This comparison highlights also that new measurements are needed to test the theoretical predictions.

Recently, the beta spectra from ^{63}Ni and ^{241}Pu decays were measured at LNHB using metallic magnetic calorimeters, with a very low energy threshold and an excellent energy resolution. The low maximum energies of these two transitions make them ideal cases for evaluating the influence of the atomic effects. The obvious disagreement with classical calculation led us to improve BetaShape by including precisely the screening and exchange effects. The latter arises from the creation of a beta electron in a bound orbital of the daughter atom corresponding to one which was occupied in the parent atom; simultaneously, an atomic electron from the bound orbital makes a transition to a continuum orbital of the daughter atom. A new screening correction is also proposed. Relativistic electron wave functions are calculated numerically, using an atomic potential generated by a uniformly charged sphere for the nucleus, including a screened potential and an exchange potential. With these precise bound and continuum wave functions, excellent agreement is obtained over the entire energy range of the spectrum for both the ^{63}Ni and ^{241}Pu decays. Statistical elements have been defined to quantify the global disagreement between experiment and theory, less than 0.05%, and the global uncertainty, of about 1%.

Finally, our recent calculation of the electron capture transitions is detailed. Allowed and forbidden unique transitions are calculated explicitly, overlap and exchange corrections are evaluated within a generalization of Bahcall's and Vatai's approaches, inner hole effect is roughly estimated using first order perturbation theory, and a rough evaluation of the shake-up and shake-off effects is also included. This model is compared to the recent high precision measurement of the second forbidden unique electron capture transition from the ^{138}La decay and to the predictions from the log *ft* program. Our preliminary results are in better agreement with the experiment than the log *ft* program and seem very promising. A systematic comparison with experimental values of both electron capture probabilities and electron capture to beta plus ratios is scheduled.

Our long term goal remains evaluating the influence of the nuclear matrix elements in order to calculate specifically the forbidden non-unique transitions.

2.5 *Improvement of ENSDF Codes (Timothy D. Johnson, Brookhaven National Laboratory, USA)*

Several upcoming directions for code development were addressed. In particular, the need to move off the Lahey FORTRAN compiler was discussed. This ties both the NNDC and users wishing to compile codes independently to an expensive vendor. For analysis and utility codes, the current state of the gfortran compiler will work, although effort will be needed to upgrade the codes to compile under gfortran and run correctly. Efforts are already underway to achieve this. In addition, for collaborative development, the GForge collaboration platform can be used. This will allow not only sharing of code development and maintenance, but versioning control, and the ability to tie in to the ADVANCE build system currently in development at the NNDC. Concurrent with this integration, unit tests need to be developed for all codes to check for quality control. These tests can be run automatically by ADVANCE after completing the build, resulting in a Web-based report.

Another issue discussed was the current slowness for the HTML rendering of ENSDF datasets on the Web. This is due to an extra security layer imposed by the Information Technology Division (ITD) at Brookhaven National Lab (BNL) on CGI code run outside the web containers. A few possible solutions were discussed. Some base cod e which can read ENSDF files and render some basic information has already been written as part of the NUDAT package, and this can be modified to present the complete content of the ENSDF file and render the standard look and feel. There exists also a Java-based publication code developed at McMaster University which currently reads an ENSDF file and converts it into a pdf file via LaTex. Although this package still needs to be brought up to speed, the code can be reused to write to an HTML file, or simply make a pdf file available on the Web. One issue involved with the pdf file option is to ensure links are done properly. As some links are dynamically generated, the approach may not be one hundred percent effective. Regardless, work will continue on the new publication code which will eventually serve as a replacement for the older publication code at the NNDC, and will be available for distribution as an alternative to ENSDAT.

It was discussed that one of the analysis codes that could be enhanced is ALPHAD. In calculating hinderance factors for alpha decay, ALPHAD currently uses tabulated radial distance (r_0) values for even-even nuclei. The evaluator must perform interpolations for

even-odd and odd-odd nuclei. The code ought to be enhanced to automate the interpolations when necessary. This could be a useful first step at fitting at least some of the analysis codes to utilize a newer language with more comprehensive library capabilities.

2.6 *A Software Development Model for ENSDF (Marco Verpelli, Nuclear Data Section, IAEA, Austria)*

This contribution deals with topics that affects the daily work of developers working with ENSDF and related software. The aim is to list few well defined issues together with a proposal for addressing them. They are grouped according to the relevance on software management, development, and design.

Software project management
A collaborative effort to develop and maintain ENSDF analysis, utility, and dissemination software would benefit from the adoption of:

- Version control system. This enables more than one person working on the same code, allows a single person to create branches for different functionalities, and provides the way to merge those developments in a single package;
- Issue tracking system. This allows to track bugs and their solutions, as well as any items deemed to be discussed; and
- Dissemination point. Software needs to be easy reachable by users, and they would also benefit in having access to discussion boards and Frequently Asked Questions pages.

The use of tools like GFORGE would provide a platform integrating the above functionalities within a project management framework.
It is worth noticing that a discussion board would benefit the network not only on software related issues. Evaluators could raise questions, track issues, build and access a knowledge base.

Software development issues
The ENSDF software development should accept contributions in Fortran, C and C++, Python, and Java since these are software languages the scientific community is heavily using, and it can be expected that valuable contributions might be offered by scientists working in one of those languages.

An Open Source-like development model, considering voluntary contributions by interested parties like students, has the advantage to increase the man-power and enrich the functionalities of the software. It should be considered advertising this opportunity on web sites like www-nds.iaea.org or www.bnl.nndc.gov.

Software design issues
The ENSDF format requires a considerable effort in parsing to extract the data to be processed by analysis or dissemination software. The input parsing, the processing, and the output generation should be 3 very well disentangled functionalities. A single, shared module should parse the ENSDF and provide a data structure to be used by other modules. This as the advantages of providing:

- a single parser to be tested;
- a place where all the unwritten rules for reading the data can be codes; and
- a module that can be disseminated to anyone that needs to process the ENSDF (for example, in producing RIPL, a considerable effort had to be put in developing the parsing).

When software needs to access data, those should not be hard-coded but provided as external modules that can be shared. This would ensure consistency and provide a single, well identified point for updating.

Considering that that the development of ENSDF relevant software is shifting from scientists-evaluators to pure software developers, it is of growing importance a software design that isolates the physics from other functionalities, and a collaboration environment the foster the communication between evaluators and developers.

2.7 *ENSDF analysis codes: Web interface and server calculations, maintenance and distribution (Viktor Zerkin, Nuclear Data Section, IAEA, Austria)*

Since 2009, the EXFOR-ENDF retrieval system has gradually been extended by so-called "Uploading" system providing a new type of service - SaaS ("Software as a service"). These systems are accessed by authorized users using a thin client via a web browser for processing their own data using software and databases on web server. The corresponding ENSDF Uploading system called 'Online Webtools' was created in 2011 and now includes the following codes: FMTCHK, GTOL, LOGFT, PANDORA, NDSPUB, RADLST. An extensive display of how the uploading system works was made. Several questions and possible ways of maintenance and distribution of FORTRAN codes, as well as requirements they have to meet with respect to documentation, standard input/output files, were presented for discussion.

2.8 *ENSDF: Feedbacks from Reaction Data (Stanislav P. Simakov, Nuclear Data Section, IAEA, Austria)*

This presentation summarises the feedbacks from analysis of decay and reaction cross section data.

Internal Conversion Electrons (ICE) spectra from decay and nuclear reactions
Recently the ICE spectrum emitted from the ^{239}Pu enriched sample was measured [2.1]. The authors compared experimental spectrum with yields predicted by the BrIcc code [2.2] and found reasonable agreement. Repeating this procedure we also confirmed this observation. However we failed to reproduce this spectrum using information available in the ENSDF database which was accessed by LiveChart [2.3]. More detailed analysis has shown that RadList code embedded in the ENSDF system correctly predicts the total ICE yield, however does not provide specific electron energies and yields for electronic subshells.

This year an advanced experiment has been carried out to measure ^{235}U(n,n')^{235m}U reaction cross section [2.4]. The ^{235m}U isomeric state has extremely low excitation energy 76.8 eV and de-excites by complete conversion in electrons with energies 42.6, 52.6 and 64.4 eV from $6p_{1/2}$, $6p_{3/2}$ and 6d subshells. Such small γ-ray energies are outside of the range of publically available BrIcc code [2.2]. Since these conversion electrons groups were obviously not resolved experimentally, the current low energy limit of BrIcc code does not result to

ambiguous interpretation of measured results. It is worthwhile to take note of the latest developments of BrIcc code which result to the extension for E3 transitions and energies below 50 eV [2.5].

International Reactor Dosimetry and Fusion File (IRDFF) and its Decay Data sub-library
In the frame of running IAEA CRP on IRDFF extension and validation [2.6] the reference Decay Library will be generated to serve as consistent decay database for dosimetry reaction evaluation and applications. At the moment it includes 88 isotopes/isomers - the unstable products of neutron activation reactions. Their important decay parameters (half-lives, decay mode, emission energies and intensities) were selected mainly from ENSDF library with some exceptional cases, where they will be taken from DDEP evaluation [2.7].

Conversion of ENSDF formatted data in the ENDF format was done by code SDF2NDF [2.8]. This procedure failed for radionuclide ^{93m}Nb. Proper modification of the conversion code is now underway.

Consistent representation of reference Atom Masses in nuclear structure databases
Calculations of nuclear reaction Q-values, thresholds, incident particle resonances energies corresponding to the unbound states of compound nucleus, cross section for inverse reaction using principle of detailed balance essentially rely on atom masses. Performing such calculations we found that nuclear structure databases or retrieval systems (LiveChart) use the atom masses values from different sources or production years. Such situation should be avoided to guarantee consistent calculation of derived physical quantities.

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2.9 *Feedback from NSDD network evaluators-Roadmap for Improvement of ENSDF Codes (Paraskevi Dimitriou, Nuclear Data Section, IAEA, Austria)*

As part of the preparatory work for the meeting and the project at large, an effort was made to collect feedback on the Analysis and Utility code used in ENSDF evaluations from all the evaluators who have in the past or are currently involved in mass-chain evaluations for the Nuclear Structure and Decay Data network. A summary of the various issues raised by NSDD

evaluators (E. McCutchan, N. Nica, A. Negret, H. Junde, S. Singh) in response to this call follows:

-ENSDAT: has problems processing a large ENSDF-type file in one go and invariably crashes.

-LOGFT: the log*ft* errors are given with a precision up to several digits which is unnecessary and does not serve any purpose.

-RULER: the code has severe limitations as it does not treat asymmetric uncertainties or values given as upper or lower limits. Also, when a level has several decay branches, the uncertainties in the transition intensity are often overestimated as a consequence of using incorrect formulas.

-EVALUATION TOOLKIT: an all-inclusive evaluation toolkit which integrates a smart user-friendly editor with the analysis and checking codes to give an output in ENSDF format and in PDF with the standard Nuclear Data Sheets style was suggested as necessary especially for the new evaluators who do not have the time to devote to or the experience to carry out mass-chain evaluations.

-AVETOOL: needs a more user-friendly interface.

-CODE MANUALS: There is a need for detailed, comprehensive manuals describing the codes, the input and output files, as well as the physics and statistical analysis models used.

Finally, the following items were suggested as important elements in the Roadmap leading to improved and easy-to-maintain ENSDF analysis and utility codes:

1. For Evaluators:
   Evaluation Toolkit: a tool that would enable the evaluator to insert all the experimental or evaluated data, process all the data using the analysis codes, check the physics and format using the checking codes, and produce a Nuclear Data Sheets style printout from the same interface without worrying about the format of the file, or how to compile and run the various codes from a command-line window.
2. For Code Developers: Certain requirements should be met when writing or modifying a code:
   a. Modern programming language
   b. Separate input/output modules
   c. Comprehensive manuals, standard input/output files for testing
   d. Portable on all Operating Systems (Windows, Linux, Mac OS)
3. Validation: the new codes will have to be tested extensively by experienced evaluators before they are distributed to the network (appropriate test cases need to be identified by validation group)
4. Dissemination:
   a. From NNDC website (and also NDS mirror site)
   b. Online Webtool
   c. GFORGE: well-suited for developers working on the development of the codes but not for dissemination to users/evaluators

3. TECHNICAL DISCUSSION

3.1 CATEGORY OF CODES AND REQUIRED IMPROVEMENTS

The codes were distinguished in three categories: Analysis, Utility (checking) and Publication Codes. Details about the functions, formats and general policies associated with these codes are given in J. Tuli's (BNL) presentation (see Appendix D).

All the codes were reviewed, one by one, with respect to bugs, deficiencies in physics models, error treatment and any other type of problem reported by participants or provided as feedback by other members of the NSDD network that were not present.

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

3.1.1 Publication Codes

The ENSDAT code that is currently used by NSDD evaluators for producing PS files in Nuclear Data Sheets style suffers from certain deficiencies. Participants agreed that the Online Webtool developed by V. Zerkin (IAEA) would be a useful tool for processing ENSDF files and producing PS without any need for installing and compiling the ENSDF codes. Alternatively, the Java Software developed by McMaster Univ., Canada could be made available to NSDD evaluators through NNDC.

Participants also recognised the importance of preserving the current display of ENSDF on the Web.

3.1.2 RULER

The program will be re-written to deal with limits and propagation of uncertainties and will include an interactive data-inputting option.

New policies were discussed and agreed upon, and they will be described in detail in the code specifications document that will be prepared and distributed to evaluators.

A new Monte Carlo method to deal with asymmetric uncertainties will be explored. Specific test cases will be developed and included in the code repository to be used for validation of the code.

3.1.3 GAMUT

A code for recommended gamma-ray energies and intensities from multiple data sets will be written following an approach similar to the previous GAMUT code that was developed at LBNL by R. B. Firestone (LBNL).

It was agreed that the problem should be developed in a step-wise approach, starting from simple averages of gamma-ray energies and intensities, with the possibility of including systematic shifts due to energy and efficiency calibration differences between different experiments. In a second step, the code will include a global matrix approach, as in GAMUT,

to obtain the recommended data. It will not however calculate correlations between uncertainties.

3.1.4 RADLIST

A new code will be written which will use conversion coefficients from BrICC and newly calculated Atomic Data on X-ray and Auger emissions. It will be further enhanced by evaluating beta spectra.

The atomic data produced by the new code will be inserted into ENSDF. In the meantime, efforts would be made by T. Kibedi (ANU) to correct the bugs reported at the meeting by M. Verpelli (IAEA) and a revised working version of RADLIST would be provided to NNDC for distribution.

3.1.5 LOGFT

The existing code will be modified to output only single-digit uncertainties in the calculated logft values.

It was recommended that the shape factors calculated by the beta spectra code developed by X. Mougeot (CEA-Saclay) be implemented in the code.

3.1.6 Checking Codes

FMTCHK: Efforts will be made to collaborate with the PNPI group to obtain an improved code for format checking.

It was recommended that the code developed by the PNPI group be included in the Online WebTool of V. Zerkin (IAEA).

PANDORA: New physics and consistency checks need to be included in the existing code.

3.1.7 ALPHAD

The Hindrance Factors uncertainties given in the output of the code should be limited to single digit.

The interpolation of the radius parameter r0 for odd-A and odd-odd nuclides should be automated. In addition, there's need to update the r0 parameters in the Akovali tables [3.1] for new half-lives, Q values from the Atomic Mass Evaluation 2012 [3.2], possible new alpha-branching ratios, and new isotopes. This is a demanding task that would require contribution from other members of the NSDD network not present at the meeting.

3.1.8 All Codes

Efforts should be made to re-structure all existing codes with the aim to separate the subroutines reading/writing input/output information from the main part of the code that performs the core operations that produce the desired output values.

Also, care should be taken so that values of nuclear parameters and/or constants that could vary in time should not be hard-wired in the main part of the code, but instead should be stored in a Common Block module or a separate library module.

These corrective procedures would ensure that keeping the codes up-to-date with current values of nuclear properties and changing formats of input files would be straightforward and almost effortless.

3.1.9 EVALUATION TOOLKIT

Participants agreed that it would be useful for the evaluators, in particular for the new and inexperienced ones, to have a compact evaluation toolkit that would integrate a user-friendly editor with the analysis and checking codes and would be available for supported operating systems.

The evaluation toolkit would provide a simple interface between the evaluator and the ENSDF file, allowing the evaluator to insert the experimental and/or evaluated values in well-defined fields without having to worry about the format. It would also allow the evaluator to run the analysis and checking codes directly from this interface without having to prepare the input file or run the code from a separate command-line window, and would also insert the results of the code directly into the appropriate fields and provide detailed error messages when necessary. The toolkit would provide a work flow to facilitate the evaluator in the evaluation procedure. This will ensure that the evaluation process is carried out by the evaluator to completion.

This compact toolkit will include the latest versions of the codes in one package and will also have the facility to check the already installed versions and update them if necessary. Efforts will be made to collaborate with authors of existing software (EVP Editor) to further enhance their capabilities according to the above requirements, ensure proper maintenance and make them available to all evaluators.

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 Programming Language and Style

The new interfaces and input/output files should be written in an easy to understand style. The programs should be adequately commented.

Standard common libraries should be created and used in the development of the different codes.

Data files used by the individual codes need to be updated and maintained in a single directory to enable continuous update.

The recommended programming languages are FORTRAN, Java, C++, and Python.

3.3 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 ENSDF Procedures Manual should be created that will integrate the existing Procedures Manual for the Evaluated Nuclear Structure Data File produced in 1987 (BNL-NCS-40503, Informal Report) and the Evaluated Nuclear Structure Data File (A Manual for Preparation of Data Sets) by J.K. Tuli (BNL-NCS-51655-01/02-Rev). This electronic manual should allow for electronic submission of revisions and keep track of the submitters, type of revision and date of revision.

3.4 VALIDATION

All codes should be rigorously tested by the code developers and experienced evaluators before distribution. This effort should be coordinated by NDS IAEA. Test cases will be defined and provided by the program developers for all operations and branches of the codes on all platforms.

3.5 DISSEMINATION OF CODES

It was recommended that the codes be disseminated in two forms, executable and source, on three operating systems, namely, Windows, Linux and MAC OS.

It was also agreed that these codes should be made available on GFORGE to enable version tracking. For this purpose a project called ENSDF Analysis Codes has been created on the GFORGE platform at NNDC, BNL. However, the official release to the NSDD network should be made only after extensive testing.

ONLINE WEBTOOL: The tool developed by V. Zerkin (IAEA) was also recognized as means of dissemination particularly as it guarantees that the ENSDF codes are available to the evaluators in their current updated version, provided they have access to the Internet. It was agreed that the new codes that meet all the requirements for dissemination will also be made available on the Online Webtool.

References

[3.1] Y. A. Akovali, Nucl. Data Sheets 84, 1 (1998).
[3.2] G. Audi, M. Wang, et al., Chin. Phys. C 36, 1287 (2012).

4. CONCLUSIONS

A new Data Development Project was 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). A Technical Meeting to define the goals and methodology of this project was held at IAEA Headquarters in Vienna, from 10 to 13 June 2014.

Participants of the meeting reviewed all the analysis and checking codes in depth, and produced a priority list of codes that need to be modified and/or re-written (see Table 1).

The nature of the improvements that need to be made were discussed in depth, responsible persons were identified and tasks were assigned with deadlines (see Table 1).

Intermediate 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 autumn of 2015.

5. LIST OF ACTIONS

Table 1. Assigned tasks.

CODES	PRIORITY	WORK	RESPONSIBLE	TIMELINE
WEBTREND/ENSDAT (EMPHASIS ON WEB RETRIEVAL)	1	REPLACE BY JAVA SOFTWARE DEVELOPED BY MCMASTER UNIV. AFTER FURTHER DEVELOPMENT	T. JOHNSON, B. SINGH	4 MONTHS
RULER	1	ADOPT AGREED POLICIES ON TREATMENT OF LIMITS, INTRODUCE PROPAGATION OF ASYMMETRIC UNCERTAINTIES	T. KIBÉDI, F. KONDEV	1ST REPORT AT USNDP 2014, FINAL PRESENTATION AT NSDD 2015
GAMUT	1	NEW CODE TO DETERMINE GAMMA-RAY ENERGIES AND INTENSITIES FROM MULTIPLE DATASETS	M. BIRCH, R. FIRESTONE, B. SINGH	1ST REPORT USNDP, PROGRESS AT NSDD 2015, BETA VERSION AUGUST 2015
EVALUATION TOOLKIT (EDITOR+CODES)	1	GRAPHICAL EDITOR INTEGRATING ANALYSIS AND CHECKING CODES	COORDINATED BY NDS IAEA: INVOLVE A. SONZOGNI	REPORT AT USNDP 2014, NSDD 2015
XLS2ENS, TXT2ENS	1	CONVERSION OF PUBLISHED TABLES TO ENSDF DATA SETS	F. KONDEV, J. CHEN, B. SINGH	USNDP 2014
ALL ENSDF CODES	1	ASSESS EFFORT AND FTE REQUIRED TO RE-STRUCTURE CODES SEPARATING INPUT/OUTPUT FUNCTIONS IN INDEPENDENT MODULES	NDS IAEA, NNDC	REPORT AT NSDD 2015
RADLIST	2	REPLACE RADLIST BY BRICC-ATOMIC AND DECAY DATA CODE	T. KIBÉDI	PROGRESS REPORT AT NSDD 2015
NEW LOGFT/BETA SPECTRA SHAPE CODE	2	USE CEA-SACLAY APPROACH FOR SHAPE FACTORS	X. MOUGEOT, NDS IAEA	REPORT AT NSDD 2015
CHECKING CODES (FMTCHK)	2	ENHANCE FORMAT CHECKING AND PHYSICS CHECKING CAPABILITIES	INVOLVE PNPI GROUP	REPORT AT NSDD 2015

PANDORA	2	ENHANCE CODE	J. TULI, E. MCCUTCHAN, B. SINGH	NSDD 2015
ALPHAD	2	LIMIT UNCERTAINTY TO ONE DIGIT	T. JOHNSON	USNDP 2014 NSDD 2015
NEW R0 INTERPOLATION CODE		INTERPOLATION FOR R0 VALUES	S. SINGH, B.SINGH	
NEW R0 TABLES		UPDATE R0 TABLES FOR NEW Q-VALUES, BRANCHINGS AND NUCLIDES	B. SINGH, S. SINGH	
VISUAL AVERAGING LIBRARY	2	PROVIDE VERSION FOR LINUX AND MAC OS	M. BIRCH, B. SINGH	NSDD 2015
NEW GABS	2	TO PROVIDE ABSOLUTE INTENSITIES FOR DECAY DATA SETS	F. KONDEV, T. KIBÉDI, E. BROWNE	PROGRESS REPORT AT NSDD 2015
LOGFT	2	LIMIT UNCERTAINTY TO SINGLE DIGIT	J. TULI, B. SINGH	NSDD 2015
ONLINE WEBTOOL	2	MAKE NEW CODES AVAILABLE	V. ZERKIN	NSDD 2015

Appendix 1

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

IAEA Headquarters, Vienna, Austria
10 – 13 June 2014
Meeting Room M0E27

ADOPTED AGENDA

Tuesday, 10 June

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
Introduction and goals of the project, P. Dimitriou (NDS IAEA)

10:45 – 12:30 **Presentations by participants**

1) Overview of ENSDF Codes and Format, J. Tuli (30 min)
2) Outstanding issues in ENSDF codes, F. Kondev (30 min)
3) Recommended Gamma-ray Energies and Intensities from Multiple Datasets, B. Singh (30 min)

12:30 – 14:00 ***LUNCH***

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

4) BrIcc and related codes to evaluate conversion coefficients and atomic radiations in nuclear decay, T. Kibédi (30 min)
5) Improved calculations of the beta-decay process, X. Mougeot (30 min)
6) Improvement of ENSDF Codes, T. Johnson (30 min)

Coffee break as needed

Wednesday, 11 June

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

7) A software development model for ENSDF, M. Verpelli (15 min)
8) ENSDF analysis codes: Web interface and server calculations, maintenance and distribution, V. Zerkin (30 min)
9) ENSDF: Feedbacks from Reaction Data, S. Simakov (20 min)
10) Feedback from NSDD evaluators, P. Dimitriou (15 min)

Coffee break as needed

12:30 – 14:00 ***LUNCH***

14:00 – 17:00 **Round Table Discussion**
Data Development Project on Improvement of ENSDF Codes
Priority list of Codes to be improved/re-written/replaced
Validation process
Assignment of Tasks/List of Actions
Follow-up meeting

19:00 ***Dinner at a Restaurant (see separate information)***

Thursday, 12 June

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

Coffee break as needed

12:30 – 14:00 ***LUNCH***

14:00 – 17:00 **Round Table Discussion (cont'd)**
Drafting of Summary Report

Friday, 13 June

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

Coffee break as needed

12:30 **Closing of the meeting**

Appendix 2

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

10 – 13 June 2014
Vienna, Austria

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Appendix 3

GROUP PICTURE

Appendix 4

Presentations

#	Author	Title	Link
1	J. Tuli	**Overview of ENSDF Codes and Format**	PDF
2	F. Kondev	**Outstanding issues in ENSDF codes**	PDF
3	B. Singh	**Recommended Gamma-ray Energies and Intensities from Multiple Datasets**	PDF
4	T. Kibedi	**BrICC and related codes to evaluate conversion coefficients and atomic radiations in nuclear decay**	PDF
5	X. Mougeot	**Calculations of beta decay**	PDF
6	T. Johnson	**Improvement of ENSDF Codes**	PDF
7	M. Verpelli	**A Software Development Model for ENSDF**	PDF
8	V. Zerkin	**ENSDF analysis codes: Web interface and server calculations, maintenance and distribution**	PDF
9	S. Simakov	**ENSDF: Feedback from Reaction data**	PDF
10	P. Dimitriou	**Feedback from NSDD evaluators-Roadmap for ENSDF Codes**	PDF

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