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# INDC International Nuclear Data Committee

## Nuclear Data Processing

Summary Report of the Technical Meeting
IAEA Headquarters, Vienna, Austria
4-7 December 2017

Prepared by

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IAEA, Vienna, Austria

January 2018

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## ABSTRACT

The Meeting was a follow-up of the Consultancy Meeting on "New Evaluated Data File Processing Capabilities", held at the IAEA Headquarters in Vienna on 5-9 October 2015. Recent progress on codes for the processing of evaluated nuclear data files was presented, including the outlook for future developments. Significant progress was made in the capabilities for generating libraries in ACE format for Monte Carlo calculations. An exercise on the verification of code capabilities for 'Generating Ace-Formatted Files' (GAFF) was endorsed. Specifications for the exercise were defined. A preliminary study was already initiated including four different codes capable of generating ACE files; additional contributions are expected from other participants.

January 2018

# Contents

# 1. Introduction

In his welcoming address, Nuclear Data Section Head, A. Koning, stressed the importance of nuclear data processing to be able to use nuclear data, because without good processing codes there is no way of using the most up-to-date nuclear data provided by the evaluators. In the past, the main processing tool used worldwide has always been NJOY, with very few alternatives being readily available. Back then, an alternative would have been the PREPRO codes but these did not have the capability of producing ACE files for performing Monte Carlo simulations using MCNP. However, this has changed over the last couple of years, mainly because NJOY 2012 was distributed directly by LANL instead of RSICC (as was the case for NJOY99) and thus less easily available. Since then, NJOY 2016 has become open source but still, the fact that alternatives are now available to users worldwide opens opportunities for verification and comparison.

A. Trkov set out the main objectives for this Technical Meeting. The availability of multiple processing codes today is a good thing because there is no longer a common mode of failure. New processing codes also mean new methods for specific tasks such as Doppler broadening, self-shielding, probability table generation, etc. A project for the verification of ACE file generation by multiple processing codes will help in the overall V&V effort of these codes. For this meeting, developers of different processing codes presented their current development status, their availability and provided an overview of the differences between MCNP calculations using ACE files generated using the newly developed processing code and using NJOY (which serves as a reference).

S. Kahler was elected Chairman and W. Haeck was elected Rapporteur by all participants.

At the adoption of the Preliminary Agenda, S. Kahler indicated that the agenda was flexible from a timing point of view, since a number of presentations had been added after circulating it among participants by email in the week before the meeting (see Appendix B).

All participants agreed to make their presentations available on the internet.

# 2. Presentations by Participants

Presentations are available at: https://www-nds.iaea.org/index-meeting-crp/TM_NDP/

## 2.1. Presentation by K. Tada (JAEA, Japan)

K. Tada presented the FRENDY code, the nuclear data processing code developed by JAEA in Japan. FRENDY is developed in C++. The development takes advantage of modern software development practices including unit testing using the Boost Test library and version control using git.

FRENDY provides a modular design in which a generic nuclear data exchange object is used for in- and output of processing modules, regardless of the original evaluation format (currently only ENDF files but support for GNDS is foreseen in the future). The processing methods implemented in FRENDY are similar to the ones available in NJOY99. NJOY99 was chosen as the reference for FRENDY because the Japanese nuclear industry and government institutions have always used NJOY99 as a base processing code.

Currently, FRENDY allows for the generation of continuous energy neutron and thermal scattering ACE files. The ACE files do not contain heating data (or kerma, which are provided in NJOY through the HEATR module) but these data are not needed when performing transport calculations in MCNP.

A first version of FRENDY will be released at the beginning of 2018, with a release to NEA member countries foreseen by the end of 2018, pending review of Japanese export control regulations.

For the comparison with NJOY, K. Tada presented a comparison of the actual ACE files for specific nuclides ($^{56}$Fe and $^{238}$U) as well as MCNP calculations using ACE files generated by FRENDY and NJOY99.

The following observations can be made when comparing the continuous energy neutron ACE files:

- The common energy grid as generated by FRENDY is finer than the one generated by NJOY.
- The number of significant digits provided by FRENDY in the output files is sometimes larger than what is used by NJOY because FRENDY uses a fixed number notation when this provides more significant digits instead of a scientific notation in the ENDF file generated by NJOY (especially for energies above 1 eV where NJOY exclusively uses a scientific notation).
- The largest differences in cross section values are observed when discontinuities appear in the ENDF source file.
- The elastic scattering cross section below 1e-4 eV is different from the one calculated by NJOY due to differences in how the cross section is approximated below 1e-5 eV for the purpose of Doppler broadening. The cross section should be assumed to follow a 1/v form or other acceptable form below the lowest energy point (typically 1e-5 eV), except for elastic scattering where a constant value should be used if Doppler broadening starts at 0 K.
- For linearization of the angular distributions by the ACER module, it has been observed that NJOY uses a reduced number of significant digits (3) which may lead to angular distributions being shifted or even being inadvertently erased.

For the thermal scattering ACE files, the following observations were made:

- For coherent elastic scattering, there is a general good agreement with the NJOY generated files. Larger than normal differences are observed at the energy boundaries.
- For incoherent elastic scattering, there is generally a good agreement but there are problems with generating the secondary energy grid from the beta grid from the thermal scattering law for liquid parahydrogen (this appears to be the only material that exhibits this issue).
- For incoherent inelastic such as ZrH, there appear to be differences in the energy grid due to linearization (NJOY does use a fixed THERMR grid of 117 points which may need improvement).

FRENDY also added improvements to the algorithm to generate probability tables for MCNP. These improvements include chi-squared random numbers and the use of the complex error function in the SLBW formalism. These changes to the algorithms do not appear to have any significant impact.

MCNP calculations were also performed using the FRENDY and NJOY generated ACE files on a select number of ICSBEP benchmarks. The keff results for both ACE file generation routes are within 0.04%. From a statistical point of view, both ACE generation paths appear to give the same results.

## 2.2. V. Sinitsa (NRC Kurchatov Institute, Russia)

V. Sinitsa presented the GRUCON code, the nuclear data processing code developed by the Kurchatov Insitute in Russia. GRUCON has been made available through the IAEA Nuclear Data Section's website (this includes the source distribution).

For the comparison exercise, ACE files were generated using GRUCON only for $^{235}U$, $^{238}U$ and $^{239}Pu$ using the CIELO evaluations. All other ACE files in the MCNP calculations were left unchanged.

For the comparison with NJOY, V. Sinitsa presented a comparison of the actual ACE files including a comparison with PREPRO as well as MCNP calculations using ACE files generated by GRUCON and NJOY.

The following observations can be made when comparing the continuous energy neutron ACE files:

- There appear to be some differences due to differences between PREPRO, GRUCON and NJOY in smoothing at the boundary of the Doppler broadened cross sections (GRUCON and NJOY agree while PREPRO differs).
- There appear to be small peaks on the MT27 cross section (this is a summation cross section, so there is an issue with one or more of the partial cross sections from which MT27 is derived, which was confirmed to be MT102).

MCNP calculations were also performed using the GRUCON and NJOY generated ACE files and no significant discrepancies were found.

V. Sinitsa also provided additional comparisons for unresolved resonance self-shielding cross sections and probability table generation. When comparing the effective cross sections in the unresolved energy range as a function of dilution, the observation is that GRUCON and NJOY UNRESR and PURR generated effective cross sections at infinite dilution agree well while the effective cross sections at lower dilution exhibit larger differences (this observation has been made by various participants of the Technical Meeting).

V. Sinitsa also looked into the generation of angular distribution data directly from the resonance parameters using the Blatt-Biedenharn formalism to determine if the difference between the generated angular distributions and the evaluator provided distributions will have an important impact on the applications. The results show that the influence on the neutron leakage spectrum from an iron sphere using a spontaneous fission Cf source documented in the ICSBEP handbook is very limited (only localized differences of the order of 2 to 3%) while the impact on the photon leakage spectrum is a lot more important (up to 80% difference).

V. Sinitsa also discussed the possibility of generating ACE files using the probability table method down into the resolved resonance region instead of only the unresolved energy region, as it has been done for fast reactor analysis in the ERANOS system.

## 2.3. L. Ping (CIAE, Beijing/CPR)

Two methods for unresolved resonance region processing are used in RULER, and the direct doppler broadening method is used for generating the ACE files in RULER.

From the comparisons of the unresolved resonance region effective cross sections and self-shielding factors between RULER and NJOY PURR, it is observed that the results of NJOY PURR are lower than those of RULER for $^{235}U$ and $^{239}Pu$, and that the differences of capture and fission self-shielding factors of $^{235}U$ are about 6% at 10 barn dilution and that the results of NJOY PURR are higher than those of RULER for $^{238}U$ and $^{241}Pu$.

From the comparisons of unresolved resonance region absorption cross sections between ENDF/B-VIII.b4 and ENDF/B-VII.1, it can be seen that the errors of resonance cross sections caused by the data library are larger than those caused by the processing code. Larger differences of $U^{235}$ capture cross sections and $^{238}U$ fission cross sections are observed between ENDF/B-VII.1 and ENDF/B-VIII.b4

From the comparisons of keff for the recommended benchmarks indicated in INDC(NDS)-711, it can be seen that most results of RULER are higher than those of NJOY PURR and it seems that NJOY PURR gives better results for the recommended benchmarks.

An older ENDF/B-VIII.b4 file was used for both $^{235}U$ and $^{238}U$ processing by RULER. The correct ACE files will be produced by using RULER at a later time, and the recommended benchmarks will be re-run against the correct ACE files. The performance of RULER will then be reanalyzed.

## 2.4. D. Lopez Aldama (AENTA, Havana/Cuba)

D. Lopez Aldama presented the URRPACK-ACEMAKER extension to the PREPRO suite of codes for the generation of ACE files for Monte Carlo calculations. The rationale behind the development of this ACE production path is the realization that the use of the same processing methods and coding reduces the probability to identify problems due to processing itself. PREPRO and the URRPACK-ACEMAKER packages are all available from the IAEA nuclear data section website.

URRPACK can calculate multiband probability tables from the original evaluated data but also from the NJOY generated probability tables which can then be reinjected in the ACE file. The resulting multiband probability tables only use 2 bins (it is not possible to change this number). A separate IAEA document is available that describes this method in more detail (INDC(NDS)-711).

ACEMAKER consists of two modules: SIXLIN to linearise MF6 and DOACE for the formatting of the resulting ENDF file into an ACE file.

$^{235}U$ and $^{238}U$ from ENDF/B-VIII.0b4 ACE files were prepared using PREPRO-URRPACK-ACEMAKER and NJOY 2012.82. The observations made when comparing the ACE files are similar to what was reported by the other participants:

- The Doppler broadened cross sections exhibit differences at the limit of the Doppler broadening region (as remarked above).
- The angular distributions look similar with some changes due to linearization of the incident energy grid.
- Delayed neutron spectra are different because NJOY adds a lower energy tail which is not added by PREPRO.

During calculations, these processing differences appear to have an impact that is generally a lot smaller than the impact of the probability tables for the self-shielding of the unresolved resonance region.

## 2.5. O. Cabellos (UPM, Madrid/Spain)

O. Cabellos gave a user's perspective on different issues on nuclear data processing. This presentation was a summary of activities presented in the JEFF Processing & Verification and Benchmarking & Validation Meetings and compiled at the NEA website (www.oecd-nea.org/dbdata/jeff/jeffdoc.html).

He reviewed the status of processing activities in the JEFF project and the processing codes used in the preparation of application libraries for different transport and burnup applications within the JEFF community. Some NJOY processing issues were presented:

- Doppler broadening with THNMAX option (in some cases Doppler broadening was stopped at a much lower energy than the user expected) – NJOY2012.82 and NJOY2016 have resolved this issue.
- Unresolved resonance region probability tables need checking for invalid or abnormal values (zero or negative cross section or zero probability values) in PURR.
- Education and training issues on processing, specifically in new evaluations of the new O-D2O thermal scattering library.
- Problems in Sn and Gd were solved by increasing allocation in ACER – NJOY2012.82 and NJOY2016.
- The MF32/RM and MLBW processing issue was fixed – NJOY2012.82 and NJOY2016.
- The legacy processing issue of $^{9}$Be covariance was fixed – NJOY2012.82 and NJOY2016.
- Processing covariances in evaluations with only MF32 – an undocumented feature of NJOY ERRORR fixes this issue by adding an empty MF33 section in an initial ERRORR run when loading the evaluation (see slide 30 in the presentation for more information, https://www-nds.iaea.org/index-meeting-crp/TM_NDP/docs/OCabellos_2017.pdf).
- Corrections were made in NJOY ERRORR in array indices, this error was detected when processing lead covariance files from JENDL-4 (taken over in JEFF 3.3).
- Long calculation times in NJOY for covariance processing defined with MF32/LRF7 formalism.
- There is a need to process additional Legendre orders and cross correlations in MF34.

The recommended options to be used in NJOY inputs for JEFF approved in the JEFF-P&V (processing and verification) working group were presented and discussed.

The impact of NJOY input options in criticality was presented using the Mosteller benchmark suite. This also identified a few benchmarks with high sensitivity to the unresolved resonance probability table (switching all probability tables on and off at the same time).

It was pointed out that proper tracking of versions and changes in different NJOY versions is important: NJOY97, NJOY99, NJOY2012 and NJOY2016. Version numbering for NJOY2016 is currently 'disabled' and should be consistently applied. Versions of NJOY that are capable of processing the latest evaluations from the ENDF/B-VIII.0 and JEFF-3.3 libraries should be identified.

## 2.6. S. Kahler (LANL, Los Alamos NM/USA)

S. Kahler presented the status of NJOY. As a first remark, S. Kahler added that NJOY2016 is now the preferred code release to be used (which is now open source, made available through github at the following address: https://github.com/njoy/NJOY2016). However, LANL recognizes that significant nuclear data activities (i.e. the ENDF/B-VIII.0 and JEFF 3.3 nuclear data libraries) are being finalized near the end of 2017 or beginning of 2018 which will impact legacy NJOY users. For this reason, LANL is offering support for NJOY2012 till the end of FY2018 (September 30, 2018).

New formats have come into play late in the game (being MF1 MT458 and MF6 MT18) – NJOY code revisions are needed to process these formats. These are currently available in NJOY2016 only and some work is still required (e.g. HEATR using new MF1 MT458 tabulated data) but these are currently not in NJOY2012.

NJOY2012.99 is currently compatible with ENDF/B-VIII.0 beta5 with the exception of the new MF1 MT458 and MF6 MT18 formats. It will produce the same ACE files as NJOY2016. Among the work to be done for NJOY2012 is the following:

- Add updates 100 and 101 (which will add updates already available in NJOY2016 due to the latest ENDF format changes)
- Develop a HEATR patch for the new MF1 MT458 tabulated energy release components
- Fix thermal scattering law NaN values that appear when running MCNP (this fix is currently being added to NJOY2016 with help from AECL/Canada). Additional work in THERMR may be required to fully resolve the issue.
- Implement other changes made in NJOY2016

The goal is to produce a final frozen NJOY2012 that is equivalent to the NJOY2016 production version when NJOY2016 is frozen. Both versions should be capable of correctly processing all ENDF/B-VIII.0 and JEFF 3.3 evaluations.

Additional work is required to provide ACE capabilities to use the new MF6 MT18 data (there currently is no place in the ACE file to put this data).

In addition, some of the covariance data proposed for ENDF/B-VIII.0 contains correlations for the angular distributions which cannot be treated by NJOY for the moment.

## 2.7. D.H. Kim (KAERI, Daejeon/ROK)

D. Kim reported on benchmark calculations for multi-band treatment of unresolved resonance region self-shielding generated by PREPRO-URRPACK and NJOY. URRPACK can calculate multiband probability tables from the original evaluated data and from the NJOY generated probability tables. The resulting multiband probability tables only use 2 bands. This is an extension of the work reported in INDC(NDS)-711.

Three types of probability tables were considered for the comparison of the selected criticality benchmarks: the standard PURR probability tables, a multiband probability table calculated from the PURR table and a multiband probability table calculated by PREPRO-URRPACK. The probability tables were generated for a selection of actinides ($^{233}$U, $^{235}$U, $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu) from two nuclear data libraries (ENDF/B-VII.1 and ENDF/B-VIII.0b4).

The keff variation is relatively small due to the use of the different types of probability tables: +/- 150 pcm with respect to the PURR probability tables for both nuclear data libraries. When comparing the two nuclear data libraries, some benchmark keff values exhibit differences that are a lot larger than the differences due to the probability tables.

## 2.8. J.-C. Sublet (IAEA, Vienna/AUS)

J.-C. Sublet presented his experience in nuclear data processing for FISPACT-II using the TENDL and other libraries. The processing path used is actually a combination of multiple nuclear data processing codes: NJOY, PREPRO and CALENDF. The NJOY processing path provides an ACE file and a multigroup file containing the DPA/kerma data from HEATR and PKA data from GROUPR. The PREPRO processing path provides a properly processed ENDF file in the high energy range (SIXPACK) and the CALENDF processing provides probability tables in the resolved and unresolved energy range. The advantage of using all three is that a cross check can be performed during the production of the library, as all three processing paths need to reconstruct and broaden the data and that multifaceted data forms are produced. The libraries are produced for 5 incident particle types: neutrons, protons, deuterons, alphas and photons.

J.-C. Sublet illustrated the content of the libraries, the resolution of the multigroup structure used in the library for specific nuclides (such as O16 MT1) and commented on specific topics such as probability table generation.

J.-C. Sublet stressed the fact that truly general purpose processed files can now be used for any application. Only some parts of the processing path will differ.

## 2.9. B. Beck (LLNL, Livermore CA/USA)

B. Beck presented the development and use of the toACE.py Python script for turning a GNDS file into an ACE file. It is part of the FUDGE nuclear data processing code under development at LLNL. FUDGE is developed mainly in Python and regular releases are made available through the National Nuclear Data Center website of BNL (https://ndclx4.bnl.gov/gf/project/gnd/). A new release is foreseen for January 2018.

FUDGE uses GNDS files as the exchange format to pass around the evaluated and processed nuclear data (all data is stored in the same file using different data "styles" to differentiate between the original evaluated and processed data). The toACE.py script takes advantage of this to transform the data into an ACE file. toACE.py currently does not have the capacity to add probability tables for the unresolved resonance region.

In addition to the toACE.py capability, FUDGE has the capability of extracting data from existing ACE files, which has helped in the development of the toACE.py capability. It has become clear that an up to date and generally available description of the current ACE format would be appreciated by the nuclear data community.

When comparing the actual files generated by toACE.py and those originating from NJOY, the FUDGE ACE files are typically larger than the NJOY ACE files. This is due to the fact that the cross sections contain more points and due to the fact that FUDGE reproduces more details in the angular distributions.

The FUDGE generation of ACE files has been tested on 5 criticality benchmarks, of which only JEZEBEL240 poses a problem (MCNP exists with an error related to $^{240}$Pu). The error message given by MCNP is related to an outgoing cosine value larger than 1.0. For the other four cases, the results produced by MCNP using the FUDGE and NJOY ACE files are statistically equivalent.

## 2.10. D. Brown (BNL, Upton NY/USA)

D. Brown presented the role of processing codes in the QA process for ENDF/B-VIII.0. He presented the evolution of the actual QA procedure used (from a pen and paper review to a fully automated system through ADVANCE). The ENDF/B-VIII.0 beta library development is now managed through the use of a subversion repository. Upon each commit, ADVANCE will run a battery of tests. The committed ENDF file will now be processed automatically by all processing codes available in ADVANCE (PREPRO, FUDGE, NJOY) and automated reports are generated, including plots, overview of messages extracted from the processing codes, integral metrics (e.g. comparisons to EXFOR), etc.

D. Brown also presented issues first presented by CEA at a WPEC SG35 meeting concerning the elastic scattering angular distribution of $^{23}$Na in which the angular distributions derived from the resonance parameters do not agree with the ones determined by the optical model, which can have a non-negligible impact on the keff value. The NNDC hosted a summer student to do two things. First, check if the angular distributions obtained through energy averaging of the angular distributions from the resonance formalisms agrees with the Hauser-Feschbach code calculated values (both methods use Blatt-Biedenharn formulas to do this). Second, repeat the exercise by assessing consistency between the angular distributions derived from the resonance parameters and the actual angular distributions in the ENDF evaluations, for the whole library. This work identified issues with Si isotopes (all Si isotopes use the same angular distributions, taken from ENDF/B-V natural Si), Cr isotopes, Ti isotopes, Pb isotopes, $^{101}$Ru, $^{105}$Pd, $^{109}$Ag, $^{108,110,116}$Cd, $^{131}$Xe, $^{133}$Cs and $^{141}$Pr.

The next step for ADVANCE is automated benchmarking. Some progress has been made in this area as well through summer student work. The system currently only uses COG Monte Carlo calculations. This is another area that will benefit from the OECD/NEA WPEC SG45 VANDAL project.

## 2.11. S. Van der Marck (NRG, Petten/NL)

S. van der Marck presented the status of automated testing of libraries available at NRG. The processing of ENDF files using NJOY is automated. This is done by using just one NJOY input file, in which some input values are parametrized (such as the ENDF MAT number), in contrast to using a database of nuclide specific NJOY inputs. The generation of ACE files is fast enough for this purpose. The generation of ACE files for roughly 300 nuclides in the benchmark inputs can be done in one night (on 10 CPUs).

The ACE files can subsequently be used in automated benchmark runs. Currently some 2600 criticality safety benchmark cases are available. The 32 benchmarks currently listed for this technical meeting are included. The results for these 32 cases based on several library versions are presented (ENDF/B-VII.1, ENDF/VIII.0 beta5, JEFF-3.1.1, JENDL-4.0).

The majority of the input files are taken from the ICSBEP DVD and Handbook, which is advised against in the ICSBEP handbook itself. A basic test is however used to check the validity of the input files: only those files are used if the input file gives the same keff result as given in Chapter 4 of the ICSBEP Handbook entry of the benchmark. If this test failed the input file was either corrected or otherwise rejected. These files have also been made available for the OECD/NEA WPEC SG45 VANDAL project.

Statistical treatment of benchmark results for keff was performed and compared to an ideal Gaussian distribution. This works quite well for the thermal and fast benchmark cases, but there appears to be a potential bias for intermediate (average lower bias) and mixed spectra (average higher bias). This kind of statistical analysis has already been applied to assess the performance of the JEFF 3.3 and ENDF/B-VIII.0 beta files.

There are possibilities to include more benchmark cases for the purpose of investigating the URR self-shielding calculations, if this is deemed worthwhile. Similarly, it could be considered to move beyond keff as benchmark values, and consider reaction rates, or shielding benchmarks.

## 2.12. C. Jouanne (CEA, Saclay/France)

C. Jouanne presented the current status of the GALILEE-1 nuclear data treatment code. The goal is to provide coherent libraries for application codes developed at CEA, being Tripoli-4, Apollo-2 and 3, depletion codes, etc.

Today RECONR, BROADR, THERMR modules are used for Tripoli-4, and UNRESR, HEATR and GROUPR are additionally used for Apollo-2 and 3. The probability tables are calculated using the CALENDF code for the whole energy range (not only the unresolved resonance range). Tripoli considers these probability tables only for the unresolved energy region.

The GALILEE code is developed in C++ and is of modular design. The internal physical data structure is very close to GNDS. The code has the following modules available for these tasks:

- Galion for input/output: read/write ENDF-PENDF-GENDF format. GNDS in XML format is to be developed
- Gbase contains the physical data object
- Galvane is dedicated to the verification of evaluation files
- Gtrend is the processing module

Today, GALILEE-1 can reconstruct 0 K cross sections for the whole energy range (this includes averaged cross sections in the unresolved resonance region), linearization can be performed in multiple ways depending on the user requirements (point by point, integral or mixed). The Doppler broadening capability implemented in GALILEE uses the SIGMA1 method for all cross sections (including threshold reactions) up to a user defined upper energy limit. Gtrend can calculate all cross sections for any energy, for comparisons with NJOY or PREPRO on the actual NJOY or PREPRO energy grid.

The GALILEE-1 system has been verified on the JEFF 3.2 library and the results appear to be in good agreement with NJOY and PREPRO.

The following differences are observed when comparing GALILEE-1 and NJOY:

- Peaks in the NJOY Doppler broadened cross sections appear for MT102 of $^{238}$U in the resolved resonance region. This observation was also made for GRUCON.
- There is no Doppler broadening above the resolved resonance region or inelastic scattering threshold for NJOY (GALILEE-1 allows this up to a user defined value, and GALILEE-1 does Doppler broadening for all reactions). Doppler broadening of the 0 K cross sections is appropriate up to the upper limit of the resolved resonance region. To Doppler broaden to higher temperatures, Doppler broadening has to be applied over the entire region of fluctuating cross sections, boot strapping from room temperature (inelastic levels and other fluctuating cross sections can also be Doppler broadened in this case).
- There is the issue of interpolation of either cross section values or resonance parameters in the unresolved resonance region. GALILEE-1 interpolates on the resonance parameters to convergence so that cross sections can be interpolated linearly within the requested tolerance. NJOY only interpolates the resonance parameters for a very coarse energy mesh.
- 9 digits in PENDF files are used by GALILEE-1.

big10 and Godiva criticality calculations performed using MCNP and Tripoli using the same PENDF files provided by NJOY and/or GALILEE and probability tables calculated by PURR (for MCNP calculations) or by CALENDF (for Tripoli4) are in very good agreement. So, as expected, discrepancies observed between PENDF files (NJOY/GALILEE-1) or probability tables (PURR/CALENDF) have no keff impact for those 2 benchmarks.

## 2.13. J. Conlin (LANL, Los Alamos NM/USA)

J. Conlin presented the current status of NJOY development at LANL. NJOY2016 is the current production version. It is a major release which includes all the improvements currently available in NJOY2012.

A major change between NJOY2016 and NJOY2012 is the code distribution model. Traditionally, NJOY has been distributed through RSICC with export control restrictions that limits the individuals that can obtain NJOY. NJOY2016 is distributed with an Open Source license with no export control restrictions. Anyone can now obtain NJOY2016 and use it for their nuclear data processing needs from https://github.com/njoy/NJOY2016.

NJOY21 is a major effort underway at LANL to modernize NJOY2016. As part of the modernization, all the assumptions made during processing (technical and otherwise) will be reevaluated.

The major goals of NJOY21 are:

- Maintain NJOY's image as a trusted and stable processing code.
- Make NJOY easier to build, verify, interact with, and process nuclear data.
- Make NJOY faster.
- Make NJOY more flexible.
- Make NJOY more maintainable.

Like with NJOY2016, NJOY21 is available without export control restrictions via an Open Source license. It is not (yet) recommended for production use, but will be made available when it is in a state that others can use it.

## 2.14. A. Trkov (IAEA, Vienna/Austria)

A. Trkov presented the current status of the ACE file verification project. The purpose of the project is to generate ACE files at 293.6 for selected ENDF files, with and without probability tables, and test these files on a selection of 32 benchmarks. Results based on the ACE files produced by NJOY (managed by the IAEA themselves), ACEMAKER, FRENDY, GRUCON, RULER and FUDGE are considered at present. For more information on these various codes, we refer to the various presentations (https://www-nds.iaea.org/index-meeting-crp/TM_NDP/). The preliminary results were presented and some issues were identified:

- ACEMAKER produced the files at 300 instead of 293.6 K.
- The ACE files produced by GRUCON were truncated through user choice at 20 MeV but this should not have any influence on the actual calculations.
- No ACE files were made available yet for FRENDY (all calculations were performed locally at JAEA)
- The ACE file produced by RULER is based on the wrong ENDF file. A new file will be provided after correction to RULER will have been made. The calculation of the benchmarks will also be performed at that time and the keff values will be reported.

C. Jouanne (CEA) has agreed to send ACE files from GALILEE-1 as well. For these last ACE files from CEA, the production path will include some modules from NJOY (PURR and ACER) while the reconstruction and Doppler broadening will be performed by native GALILEE-1 methods.

During the discussions it also became clear that identical MCNP input files for the benchmarks have to be used. A centralized repository should be put in place to ensure that every participant actually uses the same input for their testing. The OECD/NEA WPEC SG45 VANDAL project will help in this respect.

### 2.15. V. Valtavirta (VTT, Finland)

Serpent is a multipurpose 3D continuous energy MC particle transport code. It reads continuous energy neutron and photon data from ACE and uses probability tables for neutrons in the unresolved resonance region. Main applications include group constant generation (multigroup, diffusion constants, etc.) for nodal diffusion, multi-physics, fusion systems, radiation shielding, sensitivity calculations and uncertainty propagation.

Specific nuclear data treatments performed by the code itself is Doppler broadening (based on SIGMA1), on the fly temperature treatment and interpolation of thermal scattering laws.

Some questions raised related to ACE files, nuclear data evaluation and nuclear data treatments in Serpent are as follows:

- The identification of the actual isomeric state of a nuclide should be more standardized (currently the xsdir entry has modified ZA identifiers for isomeric states of the same nuclide as well as an indicator in the ACE header).
- For depletion applications, either adding MF9 and MF10 for isomeric branching ratio data in the ACE file or adding the data to a dosimetry type ACE file will avoid having to read other files.
- When generating scattering matrices, it would be good to have the energy dependent mean scattering cosines (MT251) in the ACE file as well.
- Use standardized delayed neutron groups instead of library and/or evaluation dependent group structures.
- For Doppler Broadening Rejection Correction, Serpent needs only the 0 K elastic scattering cross section. Today, Serpent needs to read the entire 0 K file.
- Serpent does not optimize the energy grid following Doppler broadening (the code actually uses the initial temperature energy grid), which may lead to significant errors.
- Runtime temperature treatments for the unresolved resonance region when using probability tables may require contributions from both transport and processing code developers.

## 3. General conclusions and recommendations

The meeting participants endorsed the ‘Generating Ace-Formatted Files’ (GAFF) exercise using independent processing codes. It will be the first time such an exercise has been set up. The GAFF exercise will provide valuable validation for the processing codes involved in the exercise and enhance confidence in the reliability of the produced libraries. The IAEA NDS expects to receive additional contributions. One such contribution has already been acknowledged, i.e. the CEA contribution using GALILEE-1, but additional contributions are welcome.

Specifications for the GAFF exercise are given in Appendix A to this report.

Extensions or follow up exercises will be proposed in a future meeting. Potential subjects include studying the influence of specific parts of the nuclear data processing, such as Doppler broadening, thermal scattering law processing, angular distribution representation, etc. Additional benchmarks including shielding and leakage can then be used to study specific aspects.

It has become clear that an up to date and generally available description of the current ACE format is needed by the nuclear data community. As this is a LANL product, an effort on their part is essential.

Generally speaking, the ACE files produced in processing paths independent from NJOY often exhibit localized differences (e.g. boundary of the Doppler broadening energy range, angular distributions, etc.). While there are differences, the use of these ACE files for keff calculations using MCNP do not lead to significant differences due to the small impact and low probability of sampling the regions in which these differences occur. The impact of whether or not using the probability tables is much larger than the impact of these differences.

Another discussion that arose during the meeting is the fact, whether or not the processing code should actually modify an evaluation when issues are detected or not (or whenever the processing code indicates that it is a concern). In some cases, this leads to differences in data between NJOY and some of the independent ACE processing paths simply because NJOY knowingly changes ENDF data to correct it. In these cases, the evaluators should be made aware of these practices. An example would be the delayed neutron spectra for which NJOY adds a low energy tail.

Such a practice can make an actual comparison of data difficult. It is recognized that an input flag should be used to allow a user to specifically turn off such corrections.

Another case for which an explicit user input flag has been requested is the reconstruction of the angular distributions from the resonance parameters using the Blatt-Biedenharn formalism. Currently, this is specifically turned off by NJOY (it is in the source code but requires recompiling NJOY to enable it). It should also be noted that the present NJOY versions only support this feature when LRF=7 is used for the resonance formalism.

## Specifications for the GAFF exercise

At the present stage, the GAFF exercise consists in generating ACE files and testing them on a collection of 32 benchmarks from the ICSBEP compilation. The selection was based on the high sensitivity to the $^{235}$U and $^{238}$U data using the NDaST software from the NEA Data Bank. The following are to be used:

- $^{235}$U and $^{238}$U evaluated data files
- ENDF/B-VII.1 and CIELO-1 evaluations as found in the "ENDF/B-VIII.0 beta4" library available from the IAEA web site https://www-nds.iaea.org/exfor/endf.htm " under "Special Libraries".
- ACE files are to be generated with- and without the probability tables.
- The ACE files are to be submitted to the IAEA co-ordinator (mailto: a.trkov@iaea.org). Normally, the benchmark calculations will be done at the IAEA to avoid input model or compiler issues.
- Calculations are to be performed using the generic ACE library based on ENDF/B-VII.1 data, with only $^{235}$U and $^{238}$U replaced by the new ACE files.
- On request the input models for the MCNP code can be provided to the participants of the exercise, noting that these are not necessarily the "best" models for the benchmarks, but merely represent the common ground for the intercomparison of the results.
- The list of ICSBEP benchmarks is given below.

| No. | ICSBEP name | Short name | Common name |
|---|---|---|---|
| 1 | HEU-MET-FAST-001 | hmf001 | Godiva |
| 2 | HEU-MET-FAST-002 | hmf002-002 | Topsy-002 |
| 3 | HEU-MET-FAST-003 | hmf003-001 | Topsy-U_2.0in |
| 4 | HEU-MET-FAST-003 | hmf003-002 | Topsy-U_3.0in |
| 5 | HEU-MET-FAST-003 | hmf003-003 | Topsy-U_4.0in |
| 6 | HEU-MET-FAST-003 | hmf003-010 | Topsy-W_4.5in |
| 7 | HEU-MET-FAST-003 | hmf003-011 | Topsy-W_6.5in |
| 8 | HEU-MET-FAST-014 | hmf014 | VNIIEF-CTF-DU |
| 9 | HEU-MET-FAST-032 | hmf032-001 | COMET-TU1_3.93in |
| 10 | HEU-MET-FAST-032 | hmf032-002 | COMET-TU1_3.52in |
| 11 | HEU-MET-FAST-032 | hmf032-003 | COMET-TU1_1.742in |
| 12 | HEU-MET-FAST-032 | hmf032-004 | COMET-TU1-0.683in |
| 13 | IEU-COMP-FAST-004 | icf004 | ZPR-3/12 |
| 14 | IEU-MET-FAST-007 | imf007 | Big_Ten(s) |
| 15 | IEU-MET-FAST-007 | imf007d | Big_Ten(detailed) |
| 16 | IEU-MET-FAST-010 | imf010 | ZPR-6/9(U9) |
| 17 | IEU-MET-FAST-012 | imf012 | ZPR-3/41 |
| 18 | IEU-MET-FAST-013 | imf013 | ZPR-9/1 |
| 19 | IEU-MET-FAST-014 | imf014-002 | ZPR-9/2 |
| 20 | IEU-MET-FAST-022 | imf022-001 | FR0_3X-S |
| 21 | IEU-MET-FAST-022 | imf022-002 | FR0_5-S |
| 22 | IEU-MET-FAST-022 | imf022-003 | FR0_6A-S |
| 23 | IEU-MET-FAST-022 | imf022-004 | FR0_7-S |
| 24 | IEU-MET-FAST-022 | imf022-005 | FR0_8-S |
| 25 | IEU-MET-FAST-022 | imf022-006 | FR0_9-S |
| 26 | IEU-MET-FAST-022 | imf022-007 | FR0_10-S |
| 27 | MIX-MISC-FAST-001 | mif001-001 | BFS-35-1 |
| 28 | MIX-MISC-FAST-001 | mif001-002 | BFS-35-2 |
| 29 | MIX-MISC-FAST-001 | mif001-003 | BFS-35-3 |
| 30 | MIX-MISC-FAST-001 | mif001-009 | BFS-31-4 |
| 31 | MIX-MISC-FAST-001 | mif001-010 | BFS-31-5 |
| 32 | MIX-MISC-FAST-001 | mif001-011 | BFS-42 |

# Technical Meeting on Nuclear Data Processing

IAEA Headquarters, Vienna, Austria
4 – 7 December 2017
Meeting Room VIC MOE16

## Preliminary AGENDA

### Monday, 4 December

**09:30 – 10:00** **Registration** (IAEA Registration desk, Gate 1)

**10:00 - 10:30** **Opening Session**

Welcoming address and Introduction – A. Koning / SH-NDS
Introduction – A. Trkov
Election of Chairman and Rapporteur
Adoption of Agenda
Administrative matters

**10:30 - 12:30** **Presentations by participants**

1. K. Tada (JAEA, Ibaraki/JPN) *(~40 min)*
   - *Comparison of the processing results between FRENDY and NJOY*
   - *Comparison of the MCNP calculations*
2. V. Sinitsa (NRC Kurchatov Institute, Moscow/RUS) *(~30 min)*
   - *GRUCON Code Package Capacities in Creating of ACE Data Files for Monte Carlo Transport Calculations*

*Coffee breaks as needed*

***12:30 – 14:00*** ***Lunch***

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

3. Ping Liu (CIAE, Beijing/CPR) *(~20 min)*
   - *Methods of self-shielding calculation used by Ruler*
4. D. Lopez Aldama (AENTA, Havana/Cuba) *(~20 min)*
   - *PREPRO/URRPACK/ACEMAKER: a system of codes to prepare ACE-formatted files for Monte Carlo Calculations*
5. O. Cabellos (UPM, Madrid/Spain) *(~20 min)*
   - *A Perspective on the Issues with Nuclear Data Processing: User´s Point of View*
6. S. Kahler (LANL, Los Alamos NM/USA) *(~20 min)*
   - *NJOY2012 – Status and Near Term Support*

*Coffee breaks as needed*

## Tuesday, 5 December

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

7. D.H. Kim (KAERI, Daejeon/ROK) *(~20 min)*
   - *Benchmark Calculations for Multi-Band Treatment of URR Self-Shielding Generated by PREPRO/URR-PACK*
8. J.-C. Sublet (IAEA, Vienna/AUS) *(~20 min)*
   - *Multi-faceted processing steps – beyond transport*
9. B. Beck (LANL, Los Alamos NM/USA) *(~20 min)*
   - *Status of creating and examining ACE files with FUDGE tools*
10. D. Brown (BNL, Upton NY/USA) *(~30 min)*
    - *The role of processing codes in the quality assurance of the ENDF/B-VIII.0 library?*

***12:30 – 14:00*** ***Lunch***

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

11. S. Van der Marck (NRG, Petten/NL) (~15 min)
    - *Automated benchmarking using NJOY & MCNP*
12. …………………………….
13. ……………………………

*Coffe breaks as needed*

## Wednesday, 6 December

**09:00 - 12:30** **Round table discussion**

- Discussion on the presentations
- Discussion on the ACE file verification exercise

***12:30 – 14:00*** ***Lunch***

**14:00 – 17:30** **Round table discussion** (cont'd)

Drafting of the Summary Report and Action List

*Coffee breaks as needed*

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

## Thursday, 7 December

**09:00 - 16:00** **Drafting of the summary report**

Finalisation of the Summary Report and Action List

**16:00** **Closing of the meeting**

*Coffee and lunch break(s) in between*

# *Technical Meeting on Nuclear Data Processing*

4 - 7 December 2017
IAEA, Vienna, Austria

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