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Technical Meeting on Processing Codes
23 – 26 September 2019

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October 2019

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Contents

1. Introduction

Arjan Koning welcomed the attendees. He noted that five to ten years ago nuclear data processing was a bottle neck, with the then current NJOY version, NJOY2012, not being as readily available as earlier code releases for generating ACE files. However, NJOY2016 and later are now open source, and there are a number of new code systems becoming available that are able to create ACE files. Code comparison exercises such as done here will make each other better. Also, multiple codes use ACE (e.g., MCNP, OpenMC, Serpent, PHITS, SuperMC) which makes another point of comparison. It is good to see collaboration tools like GitHub being used to make sharing easier.

The Chairman and Rapporteur for the meeting are:

Chairman – Tiejun Zu (China)
Rapporteur – A.C. Skip Kahler (USA)

2. Adoption of Agenda

A draft agenda had been distributed prior to the meeting. Several additional presentations have since been received and so a revised agenda, provided in Appendix A, was distributed to the attendees.

3. Administrative Matters

Andrej Trkov introduced Rosalinda Rangel Alvarez who welcomed the participants and provided administrative support for the meeting.

4. Summary of Participant Presentations

4.1 Kenichi Tada: Comparison of Processing Results of ENDF/B-VIII.0 and JEFF-3.3 Between FRENDY and NJOY2016

K. Tada presented the recent progress of FRENDY development activity and differences in the processed results between FRENDY and NJOY2016.49. The FRENDY code has been released as open source software based on 2-clause BSD license. The source code and its manual can be downloaded from JAEA website, https://rpg.jaea.go.jp/main/en/program_frendy/.

FRENDY incorporates the AMUR code to treat the R-matrix limited formula for the reconstruction of the resolved resonance region. To verify FRENDY, the (n,γ) cross section for ^{35}Cl and (n,p) cross section for ^{40}Ca from ENDF/B-VIII.0 were processed. The processing results of the (n,γ) cross section for ^{35}Cl showed good agreement with NJOY2016. However, the large difference was observed in the processing results of the (n,p) cross section for ^{40}Ca. The cause of difference is numerical instability in the Coulomb function. Compared to the other processing results, FRENDY correctly processes the R-matrix limited formula. The Coulomb function of FRENDY is taken from the JAEA optical model code POD. The Coulomb function for closed channel is calculated by the Whittaker function which is calculated by a numerical integration method.

A random sampling tool which perturbs the cross section and fission spectrum of the ACE file was developed using FRENDY. This tool can be used for uncertainty quantification with a continuous energy Monte Carlo calculation code. This tool is available in the latest version of FRENDY. A brief explanation and manual of this tool are written in the readme file and sample cases are also found in FRENDY.

K. Tada presented the difference of the processing results of ENDF/B-VIII.0 and JEFF-3.3 between FRENDY and NJOY2016. The differences were mainly observed in the comparison of ACE file generation module from the pointwise ENDF (PENDF) file.

The differences of the ACE file generation are found in precompound fraction r at DLW block, secondary energy distribution at DLW block, secondary energy distribution of prompt fission at DLW block, number of discrete photon lines at DLWP block, delayed neutron distribution ad LDND block, and decay constant in delayed neutron data ad DNDAT block. A difference was also noted in the Doppler broadening for JEFF-3.3 ^{206}Pb where NJOY zeroed small cross section values. K. Tada also noted several format errors in JEFF-3.3. These errors have been reported to NEA/Data-Bank staff. FRENDY can be used not only as a nuclear data processing code but also as a checking tool for evaluated nuclear data files.

4.2 Cedric Jouanne: Current Status on GALILEE-1 Nuclear Data Processing Code

The URR capability of GTREND was described. GTREND can produce probability tables in one of two ways:

1. NJOY/PURR-like probability tables for use with the MCNP Monte Carlo code. These tables are calculated for a number of energy points in the URR domain.
2. CALENDF-like probability tables for use with the TRIPOLI4 Monte Carlo code or the APOLLO-2 and APOLLO-3 deterministic codes. These tables are given on a multigroup energy mesh over the entire energy domain.

NJOY/PURR-like probability tables:

Here, 500,000 sets of random resonances are sampled to define the distribution of the cross sections on a given energy grid in the unresolved domain. Results for ^{238}U from the JEFF-3.2 library were presented. This nucleus contains an URR domain from 20 keV to 149 keV. The sensitivity to the number of resonances included near a given E_{res} was studied. For this, 20, 60 and 200 resonances were considered. In the case of ^{238}U, there is no obvious dependency on this parameter, but other nuclides should be studied before making a general conclusion.

As used in MCNP, we calculated 20-step probability tables from the total cross sections for these three cases. Very good agreement is obtained, regardless of the number of resonances considered.

CALENDF-like probability tables:

GTREND has the capability to produce multigroup moment-based probability tables following the method used in CALENDF. In the resolved or continuum energy ranges, moments to be preserved are calculated using the exact or the linearized cross section. In the unresolved resonance range, resonances are distributed over a domain that covers the whole unresolved resonance domain, the high part of the resolved resonance domain and the low part of the continuum, by applying the distributions defined in the evaluation files. A pointwise pseudo cross section is reconstructed in the unresolved resonance domain.

Results obtained for various calculations performed on the ICSBEP/IMF-007-2Z configuration were compared. For this benchmark, the JEFF-3.2 library was used. Calculations are performed with Monte Carlo codes MCNP-5.1.40 and TRIPOLI-4.11 with and without probability tables. The calculations include:

- TRIPOLI-4+NJOY2016 + CALENDF: pointwise cross sections and probability tables are produced using NJOY2016 and CALENDF. Calculations are performed with TRIPOLI-4;
- TRIPOLI-4 + GTREND: pointwise cross sections and probability tables are produced using GTREND. Calculations are performed with TRIPOLI-4;
- MCNP + NJOY2016: calculations are performed with MCNP and libraries are produced using NJOY;
- MCNP + GTREND: calculations are performed with MCNP. Pointwise cross sections and probability tables are produced by GTREND;
- TRIPOLI-4 + 30 random PENDF: pointwise cross sections on the whole energy domain (including

URR) are calculated using GTREND. Calculations are performed with TRIPOLI-4.

The use of probability tables in the Monte Carlo codes MCNP and TRIPOLI-4 increases the calculated k_{eff} by about 400 pcm. The TRIPOLI-4+GTREND, MCNP+NJOY2016 and MCNP+GTREND calculations are in very good agreement. The last result is the average of the k_{eff} calculated using TRIPOLI-4 with the thirty pseudo PENDF files. The average k_{eff} obtained is in very good agreement with the calculations performed using probability tables and with the expected experimental value.

Currently there is no processing for a complete library. This will be done in the near future. The GTREND code is proprietary.

4.3 Valentin V. Sinitsa: Verification of the GRUCON Modules and Computing Procedures for Group Data Processing

A complete coupled neutron-photon group data set with thermal and resonance scattering matrices has been prepared from the ENDF/B-VIII.0 evaluated data library by GRUCON (version 2019.6) and NJOY2016.49 processing codes in the VITAMIN-B6 (N199/G42) structure, for verification purposes. The GRUCON code system is available from https://www-nds.iaea.org/grucon/.

Two twin data libraries in the GENDF and MATXS formats has been obtained and compared by means of GRUCON converting and plotting modules and PLOTTAB visualization code. Typical results of comparison are presented for all data types, included to group data libraries. The maximal difference has been revealed in self-shielding factors for fissile nuclides (in the case of ^{241}Pu, ~10% at sig_0=1 barn). In the course of these analyses an unusual self-shielding factor shape as a function of dilution was observed for some nuclides (e.g., ENDF/B-VIII.0 ^{92}Mo near 40 keV). As for other group vectors and matrices, good agreement was obtained.

In addition, integral testing has been carried out through MATXS – TRANSX – MACRXS - ONEDANT calculation chain with GRUCON and NJOY processed MATXS libraries. Two types of integral characteristics have been calculated and compared:

- neutron and secondary photon leakage spectra from model shells with ^{252}Cf or 14 MeV (d,t) neutron sources at the assembly center;
- k_{eff} for critical benchmark experiments.

In the first case, a good agreement has been obtained. As for criticality calculations, unexpected and contradictive results appeared in some cases for each of MATXS libraries, pointing to inconsistencies in the transport calculation chain and not in the data processing. Additional study is needed to find and eliminate these inconsistencies.

4.4 Jeremy Conlin: ACE Capabilities in NJOY and Other Miscellanea

The ACE format was initially designed for MCNP to use the most detailed representation of the physics as practical. It has evolved along with ENDF representations for neutron and photon data. Unfortunately, the actual ACE format is a bookkeeping nightmare.
As part of the development of NJOY21 (https://www.njoy21.io/NJOY21/), LANL is creating the ACEtk component; a toolkit for working with ACE-formatted files. ACEtk - when completed - can be incorporated by other codes so they don't have to worry about the bookkeeping necessary in an ACE file. The ACE data is built up a little bit at a time to make it easier to create ACE data from other sources.

Another component of NJOY21 currently under heavy development is ENDFtk; a toolkit for working with ENDF files. ENDFtk is intended to make it intuitive to read and create ENDF-formatted data for those who are already familiar with the ENDF format.

NJOY21 is the current production version of NJOY and users are encouraged to use NJOY21 for their data processing needs. NJOY2016 is deprecated and thus will only receive bug fixes and no official development work. We have not made as much progress on NJOY21 as we would like; we had a major setback this year. However, we are working on NJOY21 as fast as resources and priorities allow.

We are aware that there are differences in the data produced by NJOY as compared to other codes. We are very interested in knowing about these differences—especially if it shows a problem in the way that NJOY processes data. If we are not notified of issues, we cannot fix them. The best way to notify us of a problem with NJOY is to file an issue on GitHub by going to https://github.com/njoy/NJOY21/issues and pushing the "New issue" button. When an issue is filed, we are notified, and we have a record of the issue and can interact with the community about it and how it can be resolved.

We have processed the ENDF/B-VIII.0 library into ACE files. These files have been heavily vetted by the Nuclear Data Team at Los Alamos to ensure they are correct. The data are available as a free download from https://nucleardata.lanl.gov. Anyone can get the data files and use them right away. This is a new way of distributing our nuclear data files and allows us to provide our data to users faster than we could in the past.

NJOY2016, NJOY21, ACEtk and ENDFtk are all open source and available at https://github.com/njoy.

4.5 Alexander Listov: Resonance Scattering Treatment in the GRUCON Package

The presentation shows the results of an evaluation of the effect of scattering on resonances in calculating the Doppler reactivity coefficient using the data preparation algorithms implemented in the GRUCON processing program. A comparison of the free-gas model with the resonance scattering model and results of calculations performed using other methods of data preparation was presented. For the Mosteller benchmark for light water grids with various fuel compositions it was shown that taking into account resonances in the differential cross sections of elastic scattering of ^{238}U leads to a shift of the Doppler reactivity coefficient by ~10% towards more negative values, meaning current methods are more conservative.

4.6 David Brown: Status of the Atlas of Neutron Resonances

The 6th edition of the *Atlas of Neutron Resonances* was published in the spring of 2018. Said Mughabghab, the author of the *Atlas* passed away on July 6, 2018. We last saw him by the end of April when copies of the new *Atlas* arrived. Said worked for more than 5 years on the new *Atlas* at no cost. While we are the inheritors of Said's work,

- Elsevier owns the copyrights to the printed copy and the PDFs;
- BNL (and therefore the US DOE) owns the electronic files.

We are working to honor Said's life's work by preparing the electronic files for eventual release, but it will take time.

We are now working on cleaning up the electronic files from which the *Atlas* PDFs are derived, carefully documenting the *Atlas* electronic format and developing a Python API for the electronic *Atlas*. This work is

complicated by the legacy formats (dating back to the days of *BNL-325*), the "hand edit" nature of many of Said's changes and occasional typos. This work was done with the help of G. Sayers, an undergraduate student from Lockhaven University.

Using this *Atlas* API, we were able to make a comparison between EXFOR and the *Atlas* bibliography. This was last done with the 2011 edition of the *Atlas* and this study was very informative. A preliminary scan of Chromium, for example, found 14 references in the *Atlas* that could not be found in EXFOR and a typo in the *Atlas* bibliography.

Another undergraduate student, S. Hollick from Rensselaer Polytechnic University, is (re)developing tools to compute the mean level spacing. The traditional approach to measuring D_0 or D_1 is to create the cumulative level distribution from all resonances with a fixed angular momentum and fit this distribution to a straight line. The slope of this line is $1/D_L$. Instead, we are overfitting the cumulative level distribution with a 6^{th} order polynomial, CDL(E), for each spin group, then computing the mean spacing from D(E) = 1/(*d*CDL(E)/*d*E). Since $D_{JLS}(E)$ should be approximately constant, larger than average spacing implies that there are missing levels while less than average spacing implies mislabeled levels. We then compared our values to the D_0 or D_1 from the *Atlas*. For ^{238}U, our polynomial method was in excellent agreement with the *Atlas* (although it can be improved much further). We also compared our method for ^{235}U. We found $D_{3,0,1/2}$=1.0 eV whereas the *Atlas* gives D_0=0.49±0.02 eV. This difference is easily tracked down to the fact that ^{235}U has two sets of s-wave resonances, with J=3 or 4 which accounts for the factor of 2 difference. However, this points to the importance of determining the provenance of all values in the *Atlas*.

We are now working to extend the *Atlas* API and implement the full set of FUDGE hooks to enable the full suite of FUDGE's RRR diagnostics.
This also allows us to complete the cleanup of the electronic files and/or implement more fault tolerant parsing. In addition, we will be rewriting the URR analysis package WRIURR which is used in
EMPIRE and *Atlas* development. WRIURR makes several assumptions about the level densities of the compound nucleus and it is not careful in its accounting for missing/mislabeled resonances. Finally, we will implement covariances (MF=32, MT=151) derived from *Atlas*. We intend to do as much of this work as possible with students.

In the longer term, we will develop methods to establish provenance of all *Atlas* quantities, a task that will likely require some combination of machine learning and SAMMY. We will work to automate this process to ensure the currency of the *Atlas* with EXFOR. Our final goal for the
Python *Atlas* API and electronic files is an open source release and possible *Atlas* web portal.

4.7 David Brown: EG-GNDS Status

Several members of the WPEC Expert Group on GNDS (EG-GNDS, https://www.oecd-nea.org/science/wpec/gnds/) are present at this Technical Meeting. This provides an opportunity to make several announcements regarding EG-GNDS. First and foremost, the specifications for GNDS-1.9 are ready! This is the first official version of GNDS released by EG-GNDS and the publication is working its way through the NEA publication system.

Future changes to GNDS are now being managed using NEA's GitLab instance (which is working quite well!), adopting a format improvement mechanism modeled on the CSEWG's ENDF Formats Committee process, but respecting NEA procedures and GitLab practicalities. To make a proposal, one must make a branch of the master git repository, make changes, then, once the change correctly builds using the NEA continuous integration system, initiate a merge request. The EG-GNDS chair and other members of EG-GNDS will nominate reviewers for the proposal and it will be up to the format proposer and the reviewers to iterate on changes until a consensus can be reached. Only once this happens and there is agreement on the format change, then the EG-GNDS chair will complete the merge request.

There are several format proposals that now must be drafted:

- New covariance format(s);
- Revised PoPs formats;
- New FPY formats;
- New documentation markups;
- New TSL formats;
- Renaming element names to clarify confusing names;
- Move `<fast Region>` out of `<background>`;
- GNDS has lots of different units, provide a mechanism to simplify it;
- Several RRR improvements were discussed, we need to make them a formal proposal.

4.8 Skip Kahler: How to Turn Probability Tables ON or OFF in MCNP

Kahler described several methods for manipulating Probability Tables (PT) when performing an MCNP6 calculation. MCNP's default action is to use PTs in the transport simulation for all nuclides that have such data. If all PTs are to be ignored, the third (iunr) variable, whose default value is zero, on the PHYS: N MCNP input card should be set to 1. This is a global change that applies to all nuclides having PTs.

To restrict the PT ON/OFF option to individual nuclides, a change in the existing ACE file and its corresponding XSDIR entry is required. Among the header data in an ACE file is an array of 32 pointers to various data. ACE format specification refers to this as the JXS array. The 23rd element of this array points to the starting location of the PTs. If this array element is set to zero, and the "ptable" text string in the corresponding XSDIR data record is deleted then the PTs for that nuclide are not used by MCNP in the transport simulation. It is important to make both changes; if only the ACE JXS (23) element is zeroed or only the "ptable" text string is deleted then MCNP will report an error condition and not execute the transport simulation.

4.9 Bret Beck: Status of URR Probability Tables and ACE File Generation with FUDGE

LLNL has developed a set of codes to handle GNDS formatted data. This includes FUDGE (For Updating Data and Generating Evaluations, https://github.com/llnl/fudge) which is a python package that allows one to generate, manipulate and process GNDS formatted data, and a suite of C++ APIs that allows access to GNDS data by transport codes. FUDGE processing generates both multi-group (for deterministic and Monte Carlo transport) and continuous energy (for Monte Carlo transport) data. The main two APIs are: 1) GIDI which reads in a GNDS file and providing access to its data, and 2) MCGIDI which extracts data from a GIDI object and puts it into a format more suitable for Monte Carlo transport. MCGIDI also supports cross section lookup, and sampling of a reaction and its outgoing particle data. The APIs have been implemented in LLNL's deterministic (Ardra) and Monte Carlo (Mercury) transport codes and tested with a suite of critical assemblies. FUDGE and the C++ APIs have been updated to support thermal neutron scattering law data and the unresolved resonance region probability tables.

FUDGE supports the conversion of the neutron data in a GNDS file to the MCNP ACE format. The conversion steps are as follows: 1) if data are from an ENDF-6 file, they can be converted to GNDS using the FUDGE endf2gnds.py script. For example

```
endf2gnds.py U235.endf U235.xml
```

2) process the GNDS file for Monte Carlo transport using the FUDGE processProtare.py. For example

```
bin/processProtare.py -mc U235.xml U235.mc.xml
```

3) run the FUDGE toACE.py script to convert processed GNDS data into an ACE file.

For example

toACE.py –i 90 U235.mc.xml U235.ace

Results of the generation of unresolved resonance region probability tables (URR-PT) at various temperatures by FUDGE were shown as well as the GNDS structures for storing URR-PT data. The results of sampling of the URR-PT data by MCGIDI were presented. Finally, results of various critical assemblies k_eff using Mercury with and without URR-PTs were presented and shown to be consistent with results from MCNP using ACE file generated by NJOY.

All codes are available at LLNL's GitHub site. FUDGE is at https://github.com/LLNL/fudge, and the APIs as well as other supporting codes are packaged into one repository dubbed GIDI-plus and is at https://github.com/LLNL/gidiplus.

4.10 Raphaelle Ichou: Current Status of the GAIA 2 Processing Code in the URR

IRSN's GAIA 1 is a wrapper for NJOY2016.35. IRSN is developing GAIA 2, a processing code which aims at being independent from NJOY. Currently GAIA 2 is an in-house code.

The following functionalities are already implemented:

- Use of Generalized R-matrix formalism for RR reconstruction;
- Reconstruction of resonances and Doppler broadening in a single step;
- Fourier transforms are used for the Doppler effect;
- Doppler effect is based on the heat equation solution.

A new thermal scattering treatment via the use of a "SAB" module is under development (based on Vaibhav Jaiswal PhD thesis), as well as the implementation of new methods for the treatment of the URR (Clément Jeannesson PhD thesis).

A new module TOP (for Table of Probability) that will replace NJOY's PURR module is being developed. TOP samples pairs (100-120 pairs are used, depending on isotopes) of resonances around a reference energy, E_{ref}, using Wigner laws, with a method analogous to the one from the PURM module of AMPX.

Sets of resolved resonances are obtained around the reference energy, and a cross section value is calculated at each iteration (10 000 iterations are used) at E_{ref}. A density of probability of cross-section values at E_{ref} is thus obtained, from which different methods are used to build a probability table. Logarithmic histogram-like, as well as equiprobable histogram-like methods can be used. The cumulative distribution functions obtained with the two methods are compared. Equiprobable binning, using a point at each 5% probability and being limited to 20 points (for use in a Monte Carlo code), has the benefit of having more points along the whole range of the cross section possible values, but it fails at representing very low and very high cross section values. Nevertheless, good agreement with the equiprobable binning method is observed with NJOY for ^{238}U total and capture cross sections.

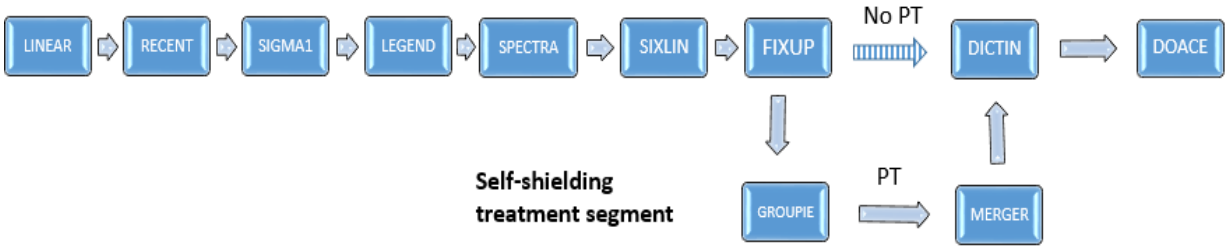
Benchmark k_{eff} calculations performed with MORET 5 show good agreement with results obtained from NJOY/PURR tables. The use of 100 binning points in ^{238}U (instead of 20) does not improve the results.

4.11 Daniel L. Aldama: Current Status of the ACEMAKER Code System for Nuclear Data Processing

ACEMAKER is a driver code to generate ACE formatted files for Monte Carlo calculations from evaluated nuclear data files in ENDF-6 format. It uses LINEAR, RECENT, SIGMA1, LEGEND, SPECTRA, FIXUP, GROUPIE, MERGER and DICTIN from PREPRO-2019 code system and two new modules SIXLIN and DOACE to process file MF6 and to prepare ACE formatted files for MC calculations.

Previously, the calculation flow also included URRFIT and GETURR from URRPACK code system, but since version 2019 of PREPRO the probability tables are calculated inside GROUPIE and the calculation flow is simplified as shown in Figure 1.

Fig. 1: Calculation flow (PREPRO-2019)



The self-shielding treatment is based on the multiband approach. The new version of GROUPIE prepares probability tables in terms of cross section data instead of shielding factors. It is recommended to use self-shielding factors, particularly if the original evaluation supplies higher resolution data for the unshielded cross section on file MF=3.

At present ACEMAKER has the following functionalities:

- Production of continuous-energy neutron data files for transport calculations including photon production in ACE format;
- Dosimetry data files in ACE format.

The code is under an extensive verification and validation program. ACEMAKER is an IAEA data development project. The source code and the manual will be released by the end of 2019 from the IAEA-NDS web site.

Soon it is planned to add the capability to produce thermal scattering data in ACE format.

4.12 Oscar Cabellos: Current Activities on Processing and Verification (P&V) at Universidad Politecnica de Madrid (UPM)

Oscar Cabellos gave a summary of recent P&V activities in which UPM is currently involved. These activities can be summarized as follows:

- In the framework of JEFF-P&V Working Group, the UPM team has performed a comparison between the FRENDY-1.01.007 and NJOY-2016.46 codes for the JEFF-3.3 nuclear data library. As a result of this work, feedback and suggested updates in several JEFF-3.3 evaluations were submitted to the JEFF Coordination Group [1]. In close collaboration with FRENDY's developers, JEFF-3.3 is processed in ACE format and successfully tested using the NEA (extended Mosteller) benchmark

criticality suite consisting of 123 cases. In a few criticality cases, differences more than three times the statistical uncertainty were found. These differences will be analysed in a future collaboration.

- UPM has been involved in the "H2020/ESFR-SMART Project" for core performance and burnup-calculations. In particular, UPM is contributing in the analyse of the discrepancies between different Monte Carlo codes for the ESFR and other fast concepts such as ASTRID, ALFD and MYRRHA. UPM was responsible for KENO-VI (package SCALE-6.2.3) calculations [2]. A comparison of KENO-VI results with SERPENT and MCNP6 codes showed an issue in the unresolved resonance region (URR) processing with the AMPX code. AMPX overestimates the production cross section while capture is underestimated. This feedback was submitted to SCALE developers, the issue has been fixed and will be included in the next SCALE (6.3.0) release.
- In the area of Nuclear Criticality and Safety, UPM is participating in the WPNCS Sub-Group 3 on "The effect of temperature on the neutron multiplication factor for PWR fuel assemblies" [3]. A summary of MCNP-6.1 calculations performed by UPM was presented. This benchmark has served to show i) the necessity of a S(α,β) interpolator, ii) the impact of NJOY options for the generation of thermal ACE files (number of angular bins in THERMR and energy bins in THERMR) in k_{eff}, and iii) the differences in k_{eff} using different nuclear data evaluations. In this work, ENDF/B-VII.1, ENDF/B-VIII.0, JEFF-3.1.1 and JEFF-3.3 were compared [4]. Regarding the effect of temperature in criticality, a comparison of calculations for the "Computational Benchmark for the Doppler Reactivity Defect" proposed by R.D. Mosteller in 2006 was also shown [5].
- Finally, a PWR core analysis is presented for a Spanish PWR unit using the SEANAP system, a computational system for the 3D core analysis of the Spanish pressurized water reactors. JEFF-3.3 and ENDF/B-VIII.0 were processed into WIMS-D format and used to upgrade the SEANAP system. SEANAP showed excellent predicting capabilities for the critical boron concentrations (in ppm) with the measurements within a factor of 20-50 ppm. In addition, an Uncertainty Quantification (UQ) analysis was also performed showing that the main contributions to the uncertainty in the prediction of boron concentration are the uncertainties in the cross-sections and nubar of ^{235}U and ^{239}Pu, an uncertainty value of 40-70 ppm is predicted [6].

References:

[1] JEFF-JENDL Bilateral Meeting, "First feedback on using FRENDY for processing of JEFF-3.3.", O. Cabellos. April 24, 2019. NEA Headquarters.

[2] "About the impact of the Unresolved Resonance Region in Monte Carlo simulations of Sodium Fast Reactors", A. Jiménez-Carrascosa et al., ICAPP 2019 – International Congress on Advances in Nuclear Power Plants, France, Juan-les-Pins, May 12-15, 2019

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[4] JEFDOC-1953, "WPNCS-SG3 Benchmark on the Effect of Temperature on the Keff for WPR Assemblies: UPM Preliminary Results", O. Cabellos. November 2018.

[5] JEFDOC-1953, "Computational Benchmark for the Doppler Reactivity Defect: UPM Preliminary Results", O. Cabellos. November 2018.

[6] JEFDOC-1968, "Comparison of JEFF-3.3 and ENDF/B-VIII.0 in PWR simulations ", A. Ardura et al., April 2019

4.13 Ville Valtavirta: Topical Issues with Serpent and Evaluated Nuclear Data

Dr. Valtavirta from VTT presented the current relationship of the Serpent Monte Carlo code and evaluated nuclear data. The code currently transports neutrons and photons. The current applications of the code range from traditional reactor physics to more general radiation transport also including sensitivity/uncertainty analysis. The most recent nuclear data needs have been related to dosimetry data (current version is IRDFF-v1.05; IRDFF-II will be released by the end of 2019), incident neutron heating data (MF=1/MT=458 data + KERMA coefficients), incident neutron photon production data (from ACE-files), incident photon nuclear reaction data (also from ACE-files) and covariance data for uncertainty quantification applications.

Dr. Valtavirta presented preliminary Serpent results for the 32 ICSBEP benchmark collection (see Appendix B) for the ACE-verification project obtained with ^{235,238}U evaluations from ENDF/B-VIII.β4 and the rest of the nuclides from ENDF/B-VII.1.
The presented results switched probability table sampling off and on for all nuclides. The PT-off results will be recalculated with only ^{235}U and ^{238}U probability table sampling turned off (other nuclides on).

Finally, Dr. Valtavirta noted that photonuclear interaction modelling has been recently implemented into Serpent with a conference paper on the topic presented in M&C2019. The photonuclear interaction data is read from ACE-format files. Initial verification has been conducted against MCNP-6.2 and TRIPOLI-4 with ENDF/B based data (endf7u library for Serpent and MCNP). During this verification some problems were noted in the incident photon data:
* ENDF/B-VII.0, VII.1 and VIII.0 (all contain the same data)
- Angular distributions are not given for MT=50-71 reactions (discrete two-body reactions) in ^{182,186}W (also missing from MCNP's endf7u photonuclear library);
- In ^{9}Be, a discontinuity exists in the cross section of MT=29 reaction (n+2α) at 20.0 MeV;
- Suspiciously high photon product yield (161.2955) at 8.7 MeV in ^{36}Ar (maximum yield at other energies is 3).

❖ TENDL-2017
- Poor agreement with ENDF/B and JENDL/PD-2016 libraries and experimental data in ^{9}Be.

4.14 Liu Ping & Wu Xiaofei: Development of a Probability Table Generation Module

In the development of probability tables generation module PURD, the ladder method is used to generate probability tables. The ψ-χ formulas are used to calculate the cross sections, including capture, fission and elastic scattering cross sections. The continuous random number generator is used to generate Chi-Squared random numbers. Comparison of probability tables for ^{235}U has been done for RULER, NJOY99 and NJOY2016, and the difference was not significant. Because of parallelization in the probability tables generation in PURD, the running time of PURD is faster than that of PURR of NJOY. The RULER code system is currently an in-house code of the CNDC and Tsinghua University.
In order to test the module PURD, the verification of ACE files with probability tables based on ENDF/B-VII.1 data has been done. The 32 benchmarks recommended in Stage-1 were used to do the verification of ACE files. The verification results are compared between ACE files with probability tables and ACE files without probability tables. It can be seen that the k_{eff} values of benchmarks from ACE files with probability tables are closer to those of NJOY, and the differences from NJOY are not large except for the IMF22-6 benchmark. The difference needs further analysis and verification. It indicates that the probability tables are necessary.

4.15 Jialong Xu: Progress of the Development of the Nuclear Data Processing Code NECP-Atlas

NECP-Atlas (http://atlas.xjtu.edu.cn) is a nuclear data processing code developed by Xi'an Jiaotong University in China.

The code has been tested against various evaluations, and can produce different format libraries, such as ACE, WIMS-D and MATXS. The ladder sampling method is used for the unresolved resonance region. We have done many sensitivity analyses to decide the parameters for the generation of probability table. The computation efficiency is improved by using a faster (quick sort) sorting method.

There are some improvements in the calculation of effective cross sections in the unresolved resonance region. The interference effect caused by the overlap of resonances in each resonance sequence is considered. Meanwhile, the interference effect caused by the overlap of different resonance sequences is taken into consideration. A function module to treat resonance elastic scattering effect is included in the code and tested with several benchmarks.

A multi-point linearization method is used to adaptively generate incident energy grids for S (α, β) tables.

Adaptive linearization is used to linearize the cross sections.

4.16 Andrej Trkov: Code Validation for Generating ACE Libraries

Following the request of the IAEA Member States, the IAEA initiated an activity to provide a data processing system independent of NJOY, which was not generally available at the time.

With the IAEA support the ACEMAKER code was developed. It makes use of the PREPRO codes for basic operations and assembles the ACE file. The recent updates by D.E. Cullen in PREPRO-2019 are gratefully acknowledged; they greatly simplify the processing procedures.

In the meantime, seven other codes became available. In total, there are nine codes:

NJOY – USA
FUDGE – USA
GRUCON – Russia
FRENDY – Japan
ACEMAKER/PREPRO – IAEA
NECP-Atlas – China
RULER – China
GAIA – France
GALILEE- France

The ^{235}U and ^{238}U evaluated data files from ENDF/B-VIII.β4 were chosen for testing. ACE libraries for ^{235,238}U provided by the participants were tested. 32 criticality benchmarks from ICSBEP were considered (same as for Stage-1, https://www-nds.iaea.org/ACE_verification/).

Results for 9 codes were available:
3 codes agree with NJOY to within ~ 20 pcm; how independent are they from the methods of NJOY?
5 codes agree with NJOY to within ~ 150 pcm; reasons for the differences are to be investigated.

Detailed results are available on the Meeting web page (https://www-nds.iaea.org/index-meeting-crp/TM-Nuclear%20Data%20Processing/)

It was agreed that the participants would provide a one to two-page description of the resonance treatment in the unresolved resonance range for the purpose of assembling a paper for publication in a journal.

5. Recommendations and Action Items

1. Create a journal paper with results and with each code system's URR method explained. Also discuss differences in the calculated k_{eff}. No one code is the reference, use average with individual deviations.

ACTION 1: Coordination of this paper to be done by the IAEA Nuclear Data Section;
ACTION 2: All code authors to send a one-to-two-page description of the main features of the URR treatment in their codes to the IAEA.

2. Meeting participants and other interested parties should send their latest ACE files to the Agency for a final set of MCNP criticality calculations.

ACTION: all code authors.

3. In the longer term the Agency should consider similar exercises for
    a. thermal neutron scattering law data;
    b. photon production data;
    c. charged particle production data;
    d. dosimetry data;
    e. photo-nuclear data;
    f. photo-atomic data;
    g. incident charged particle data.

ACTION: all code authors to provide information about their code's capability to process these data and produce ACE files, and to report on the status of the ACE format documentation for each of the above items.

4. Heating (KERMA), damage and gas production processing capability are needed in other codes. For example, the fusion community (FENDL users) has an increasing interest in Damage.

ACTION: all code authors to report on the Heating and damage calculation capability in their respective codes.

5. A more complete ACE format document that includes charged particle production, photo-atomic and photo-nuclear specifications is needed.

ACTION: participants are encouraged to submit format descriptions to https://github.com/NuclearData/ACEFormat.

Appendix 1: Agenda

EVT1805452

Technical Meeting on Nuclear Data Processing

IAEA Headquarters, Vienna, Austria
23 - 26 September 2019

Meeting Room M0E79

AGENDA

Monday, 23 September

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

09:30 **Opening Session**

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

09:30 - 12:30 **Presentations by participants** (~ 20 to 30 min)

Kenichi Tada: Comparison of processing results of ENDF/B-VIII.0 and JEFF-3.3 between FRENDY and NJOY2016

Cederic Jouanne: Current status on GALILEE-1

Valentin V. Sinitsa: Verification of the GRUCON modules and computing procedures for group data processing

Jeremy Conlin: ACE Capabilities in NJOY and Other Miscellanea

Coffee break as needed

13:00 – 14:30 ***Lunch***

14:30 – 17:30 **Presentation by participants** (~ 20 to 30 min)

Alexander Listov: Resonance scattering treatment in the GRUCON package

David Brown: Status of the Atlas of Neutron Resonances

David Brown: EG-GNDS Status

Coffee break as needed

Tuesday, 24 September

09:00 - 13:00 **Presentations by participants** (~ 20 to 30 min)

Raphaelle Ichou: On the treatment of URR data in GAIA

Daniel L. Aldama: Current status of ACEMAKER code system for nuclear data processing

Oscar Cabellos: Current activities on Processing and Verification(P&V) at Universidad Politécnica de Madrid (UPM)

Ville Valtavirta: Topical issues with Serpent and evaluated nuclear data

13:00 – 14:30 ***Lunch***

14:30 – 17:30 Presentations by participants (~ 20 to 30 min)

A. (Skip) Kahler: Turning On/Off probability tables in ACE

Andrej Trkov: Results of the intercomparing of codes for generating ACE files for incident neutrons above the thermal energy range

All: Discussion of the results

Coffee breaks as needed

19:00 ***Dinner at Restaurant "Kolariks"***

Prater 128; Waldsteinergartenstrasse

Wednesday, 25 September

09:00 - 12:30 **Discussions by participants** (~ 20 to 30 min)

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **Drafting of the final report**

Coffee breaks as needed

Thursday, 26 September

09:00 - 16:00 **Finalization of the report**

16:00 **Closing of the meeting**

Coffee break(s) and lunch in between

Appendix 2: Participants List

Technical Meeting on the Nuclear Data Processing

23 to 26 September 2019
IAEA, Vienna

List of Participants

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Appendix 3: List of benchmarks used in the ACE Library Verification exercise

.	ICSBEP Label	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

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