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Nuclear Data Processing

Summary Report of the Technical Meeting
18-22 October 2021
(virtual event)

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January 2022

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1. Introduction

Opening Remarks

Arjan Koning: The situation for processing codes is healthier than ever before. In the past, only PREPRO and NJOY were available. Now, with new initiatives all over the world, there are at least six new fully operational processing codes for fast and thermal neutron transport, and three more doing a partial job. From the meeting agenda, one can easily see the increased interest in the thermal scattering law (TSL) for neutrons and related data processing. The next versions of the evaluated libraries will not be available before at least one year and a half, which means that there is some time for further development of the processing codes.

Roberto Capote: These days, it is becoming more and more important to put together evaluators and users. There is a spread of 300-500 pcm (parts per 100 000) in predicted benchmark reactivity among processing codes due to the choice of initial parameters and thresholds. Some specific features are defined internally in the processing codes. It is necessary to make comparisons with experimental data in order to recommend both an evaluation *and* its specific processing. Differences from nuclear data processing codes are expected to be a maximum of 20-30 pcm to be comparable with a typical statistical uncertainty of Monte Carlo calculations.

Election of Chair and Rapporteur(s)

Andrej Trkov was designated chairman with unanimous assent.

Andrej suggested sharing the role of rapporteurs among different participants.

Monday: Daniela Foligno, Skip Kahler; Tuesday: Daniela Foligno, Skip Kahler; Wednesday: Oscar Cabellos, Wim Haeck; Thursday: Wim Haeck; Friday: Skip Kahler.

2. Presentations by Participants

2.1. Current achievements of the code verification project for generating ACE libraries, A. Trkov (JSI)

In the last few years, a lot of effort was put into checking processing codes used to produce ACE files for Monte Carlo codes. This was done in three stages.

Stage 1 consisted in verifying the processing of cross sections and energy/angle distributions without self-shielding. Nine codes were tested: NJOY, FUDGE, GRUCON, FRENDY, ACEMAKER/PREPRO, NECP-Atlas, RULER, GAIA, and GALILEE. The test case was to process ^{235}U and ^{238}U from ENDF/B-VIII.b4. A number of benchmarks from the ICSBEP Handbook were identified for the analysis. All the codes could process the cross sections within the specified tolerance. Most results agreed within 20 pcm. Results can be checked on the IAEA webpage (http://www-nds.iaea.org/ACE_verification/).

Stage 2 included self-shielding in the calculations. Self-shielding in the resolved resonance range (RRR) is treated explicitly, but methods for generating probability tables in the unresolved resonance range (URR) might be different from code to code. By selecting benchmarks that are particularly sensitive to the URR, it was possible to analyze the processing capabilities of certain codes. The discrepancies did not exceed 100 pcm. Considering the uncertainty in the benchmark experiments, the results can be considered acceptable, but since this is essentially a numerical exercise, it is highly desirable to decrease the differences further down to 20-30 pcm. It would be worthwhile for the authors of the codes to investigate

the reasons for such discrepancies. Unfortunately, even with high sensitivities, the uncertainties in the experimental integral benchmarks are so high that it is impossible to single out those codes showing the best performance.

Stage 3 consisted of testing the processing of TSL in order to have all the elements to analyze thermal systems. The test case was H in ZrH from ENDF/B-VIII.0. The benchmarks were selected from the ICSBEP cases containing ZrH. There are two ways of representing the data in ACE (defined by the IFENG flag), and it is important to check their impact on the results. Ten benchmarks were tested. Contributions came from all over the world using different codes (NJOY, ACEMAKER/PREPRO, NECP-Atlas, FUDGE, FRENDY, GRUCON). The first observation concerns the difference between IFENG 1 and 2. The format description for IFENG=2 only became available recently. The differences in the results for different IFENG options are relatively small, but for the HEU-COMP-MIXED-003 Case-1 benchmark, it exceeds 200 pcm. This is only due to formal representation of the data, and it is an undesirable feature. In general, IFENG=2, which was developed later and features continuous outgoing particle energy distribution, should be preferred. Among codes using IFENG=2, there are other different features (e.g., upper energy for the TSL treatment, energy grid of the incident neutron in materials like metal hydrides that exhibit oscillatory behaviour, number of cosine bins). The results indicate that it is necessary to consider thermal neutron up-scattering up to 4 eV, or even as high as 10 eV. The upper energy of thermal scattering seems to be more important than expected. The codes give results within 50 pcm from each other.

It is also important to highlight that ENDF-6 format extension was approved for TSL to allow both, coherent and incoherent elastic cross section representation, and processing codes will need to be upgraded to consider mixed coherent and incoherent elastic scattering.

Considering the observed differences in the results of Stage-2 that included self-shielding effects, the discussion on self-shielding continues. It is impossible to discriminate, using the criticality benchmarks, which way of treating self-shielding cross section is more accurate. At RPI, an experiment on transmission yield from a thick tantalum target was performed and could be used as a benchmark.

Q&A, comments, discussion:

B. Beck: FUDGE can handle this new format. Is there a way to put it into ACE?

A. Trkov: Can you create it? MCNP was upgraded to use this.

J. Conlin: Wim will talk about this later.

P. Romano: (chat): the proposed ACE format changes can be found in:

<https://github.com/NuclearData/ACEFormat/pull/23>

R. Capote: The actinide group in INDEN was discussing about the impact of URR, and Yaron Danon and coworkers at RPI proposed a transmission experiment to be a benchmark. The main conclusion is that there is not only the impact of the quality of the evaluation, but also of the data processing. It also depends on the format of the library. Despite the fact that there is agreement on the URR processing within 100 pcm, what is even more important is to check the agreement with the experimental/measured data. We need that. In the particular case of URR, my feeling is that we have to take a common approach (evaluators and users).

W. Haeck: the document is not finalized yet, but the TSL format as it is implemented in NJOY and used in MCNP won't change anymore. It is finalized.

A. Trkov: Can MCNP interpret this new format?

W. Haeck: MCNP 6.3 yes. The only issue is that I only have one evaluation that uses this format. I used the example file that was used in the format change proposal.

S. Kahler: Is there a schedule after MCNP 6.3?

W. Haeck: For the moment only bug fixes.

S. Kahler: What happens right now if you use the previous version? Does it crash?

W. Haeck: Not tested yet. MCNP checks what type of ACE file it is (incoherent or other). It is possible that the code will only use the coherent part and ignore the incoherent part.

O. Cabellos: Can you recommend the IFENG flag? It is not in the manual.

A. Trkov: IFENG=2 was introduced because the old one used discrete outgoing particle representation. It makes spikes in the spectrum, which are unphysical. IFENG=2 makes the spectrum continuous.

K. Tada (chat): In the ACER module, IFENG is an IWT option. IFENG=1 means IWT=0, while IFENG=2 means IWT=2

O. Cabellos: in the manual, the default option is IWT=0, therefore IFENG=1

A. Trkov: the default option should be changed.

2.2. Processing thermal scattering law and dosimetry files for Monte Carlo calculations using ACEMAKER, D.L. Aldama (IAEA)

The processing code system ACEMAKER has been updated by including the capability for preparing thermal and dosimetry ACE-formatted files.

The new module DOTSL processes the thermal scattering law given in ENDF-6 format. It can handle the inelastic scattering as well as the coherent and incoherent elastic scattering, including the new so-called mixed TSL format.

An initial dense incident energy grid is built for processing the inelastic scattering. Afterwards, a thinning procedure is applied based on the tolerance specified by the user. The outgoing energy grid for each incident energy and the required cosines grid for each outgoing energy are adaptively prepared in such a way that the corresponding distributions can be linearly interpolated. The initial grids for the outgoing energies and cosines are built from the tabulated values of the dimensionless energy and momentum transfers, respectively. The DOTSL module always uses the continuous representation of the inelastic scattering (IFENG=2), giving the probability distribution and the cumulative distribution of the outgoing energy for each incident energy. The angular distribution is represented by a set of equally probable cosines. These probability distributions and cosines are calculated from the linearized energy and angle distributions. Finally, the cumulative distribution is thinned by removing very small differences which mainly impacts the values very close to 0 or 1.

For the incoherent and coherent elastic scattering, analytic expressions are used to calculate the required cross section and angular distribution (incoherent case). A set of benchmarks was successfully analyzed for verifying and validating the code. Additionally, studies included the impact of cutting the thermal energy range, the number of incident energy points and the number of equally probable cosines on the benchmark results. It was found that a relatively dense incident energy grid is needed between 0.001 eV and 2.85 eV for moderator materials with an oscillating cross section in this region like the hydrogen in ZrH. It was also important to extend the thermal scattering treatment to 4.0 eV or more. Furthermore, a value of 32 equally probable cosines was found adequate for most moderators.

On the other hand, the module DODOS of ACEMAKER was updated for processing dosimetry files. The dosimetry cross sections can be obtained from the cross sections included in the files MF3 and MF10 or from the yields given in the files MF9 or MF6 and the cross sections stored in the file MF3. The processing of natural elemental composition targets was added as a new capability.

The newly released package ACEMAKER-2.0 is able to produce fast, thermal and dosimetry ACE-formatted files from ENDF-6 formatted evaluated nuclear data files for Monte Carlo simulations. New developments are ongoing to add the capability to process photonuclear data and charge particles production data.

2.3. Treatment of thermal scattering law data in FRENDY, K. Tada (JAEA)

K. Tada presented the processing of the thermal scattering law data in the FRENDY code and described recent activities.

The processing method of the FRENDY code is similar to that of the NJOY code. The main difference is the number of energy grid points generated. The energy grid of FRENDY is obtained from the Doppler broadened PENDF file of the nuclide, which is finer than the NJOY energy grid. Compared to the NJOY code, larger differences are found in the cross section when it exhibits oscillating behaviour.

K. Tada reported some problems of the NJOY code. The characteristic difference between the FRENDY code and the NJOY code is observed in para-H, ortho-H, para-D, and ortho-D from JENDL-4.0 where the incident neutron energy is less than $1.0E-3$ eV. The cause of the difference is the treatment of the outgoing particle energy in the NJOY code. The NJOY code skips the calculation of the inelastic scattering cross section when the incident energy is identical to the outgoing particle energy. The initial outgoing particle energy grid of the NJOY code is the energy grid of the beta parameter. When the minimum energy grid of the beta is identical to the incident neutron energy, the linearization of the outgoing particle energy grid distribution from the lowest energy to the incident neutron energy is skipped. This outgoing particle energy treatment affects the cross section in the low energy region.

The largest energy grid of the THERMR and the ACER modules of the NJOY code are different even if the maximum energy (EMAX) in the input file is identical. If the user sets EMAX=5.0 eV, the largest energy grid of the THERMR module is 5.35 eV and that of the ACER module is 4.90 eV.

The IWT option in the ACER module (the IFENG flag in the ACE file) shows the representation of the angular and the outgoing particle energy distributions. Though the recent official ACE file uses IWT=2 (IFENG=2), MCNP6.1 and earlier versions sometimes terminate execution prematurely. The cause of this problem is the narrow width of the outgoing particle energy grid. In the calculations MCNP makes use of the inverse of the secondary energy grid width. If the outgoing particle energy grid width is so small, e.g., $1.0E-17$ MeV, the inverse of the outgoing particle energy grid width becomes infinite. The FRENDY code does not add new outgoing particle energy grids when the minimum distance is less than $1.0E-14$ MeV to avoid this problem.

The FRENDY code also prepares the checking function of input parameters (i.e., "NATOM" of the THERMR module and "NMIX" and "IELAS" of the ACER modules). The FRENDY code checks the processing results to verify these input parameters since they have a large impact on the processing results. These checking functions are helpful to make the proper input file.

Recently, K. Tada and his colleagues developed the neutron induced multi-group cross section generation function and uncertainty quantification of the probability table. The next version of the FRENDY code, i.e., FRENDY version 2, will be released including these functions by May 2022.

Q&A, comments, discussion:

W. Haeck: NATOM and NMIX are often the cause of issues. These values were originally not given in the evaluations, which is why they need to be given in the NJOY input file. These values should be read from

the evaluations if they are given.

T. Zu: We tested the incident energy grid. Sometimes it can introduce more than 100 pcm difference on the k_{eff} of some benchmarks.

K. Tada: It depends on the materials.

A. Trkov: Did you test the impact of the upper energy?

K. Tada: This energy region has no impact on the short-collision time approximation.

A. Trkov: TSL data go up to 1.8 eV, and after that, you use short-collision time approximation. Should we recommend the evaluators to go to higher energies in the TSL evaluation or is the SCT approximation good enough?

K. Tada: We need higher energy $S(\alpha, \beta)$ data.

V. Sinitsa: What is the diagnostic of MCNP when it fails due to the energy grid?

K. Tada: From MCNP-6.2 on, if the energy grid becomes very narrow, the linearization of energy grid is skipped and the simulation does not fail. MCNP-6.1 computes $(E'_i + 1 - E'_i)$ before the calculation of $1 / (E'_{i+1} - E'_i)$. When the value is too small, MCNP-6.2 does not compute the ratio, while previous versions fail.

2.4. Capabilities of the GRUCON code package in the TSL data processing, V. Sinitsa (NRC Kurchatov Institute)

The GRUCON modules dedicated to the processing of ENDF-6 MF7 files are described. Various cross section representations can be used for preparing the ACE file, namely:

- fixed/adaptive energy grids for incident neutrons,
- discrete equally-probable cosines,
- discrete, equally-probable energies obtained with constant or variable (skewed) weights, as well as continuous energy distributions of scattered neutrons. 132 materials from the ENDF/B-VIII.0 data library have been processed with the NJOY2016.62 and GRUCON-21 codes to produce continuous energy ACE files. Thermal ACE files for H in H₂O, Be metallic, Be in BeO, O in BeO, C in graphite, H in ZrH and Zr in ZrH were also created, using the options noted above.

The obtained files were used for comparison at differential and integral levels, by comparing k_{eff} values calculated for a set of ICSBEP benchmarks. Comparison of inelastic incoherent cross sections obtained at fixed and adaptive energy grids reveals a disagreement in the cross sections of up to 6% (in the case of H in ZrH) due to interpolation errors. At the same time, comparison of incoherent elastic and coherent elastic cross sections and energy/angular distributions did not show any discrepancies that could affect integral results.

For integral comparison, 87 benchmarks with thermal and intermediate spectra have been selected from the ICSBEP Handbook and k_{eff} calculations have been performed by MCNP with three ACE libraries:

ACE_NJOY	Library with files, generated by NJOY;
ACE_GRUCON	Library with files, generated by GRUCON;
ACE_MIXED (TSLMAT)	Library with files from the ACE_GRUCON library except for one TSL file taken from the ACE_NJOY library.

The comparison showed agreement to within ± 100 pcm in k_{eff} for all runs with ACE_MIXED and ACE_GRUCON libraries, showing the impact of the differences in the TSL processing. As for comparison of ACE_NJOY and ACE_GRUCON calculations, there is only one case of disagreement of ~ 200 pcm (HEU-COMP-MIX-003 Case-1), probably caused by the accumulation of errors from ACE files with fast neutron

data (55 isotopes for this benchmark). A systematic shift of all curves, obtained in the PU-SOL-THERM (minus ~50 pcm) and MIX-COMP-THERM (plus ~50 pcm) benchmark sets requires additional study.

Q&A, comments, discussion:

D. Aldama: What difference did you find in k_{eff} when you were using IFENG=1 with respect to IFENG=2?

V. Sinitsa: Depends on the lattice.

2.5. TSL data processing for MCNP in KAERI, D.H. Kim (KAERI)

There has been an increased need for ACE temperature data for different applications (research reactor, micro reactor, material science). Special attention was given to TSL temperature data. The research reactor group required TSL data (H_2O , Be, BeO, D_2O , graphite, CH_2) at 18 temperatures. The Nuclear Data Validation Group of KAERI/NDC produced the base ACE library from ENDF/B-VIII.0 to make the KNE80 library. It also produced the TSL library from ENDF/B-VIII.0 to make the KNE80SAB library. Temperature data were produced using the LEAPR inputs provided in the ENDF/B-VIII.0 package. There is a fixed phonon frequency spectrum for all temperatures except for H_2O and D_2O . D.H. Kim showed the interpolated and extrapolated phonon frequency spectrum for H_2O and D_2O at 18 different temperatures. The research reactor group gave feedback on TSL, concluding that the system would be safe with these parameters. D.H. Kim showed some criticality benchmark calculations (64 problems from the expanded criticality validation suite, 12 from ICSBEP, but only one for the ZrH case). The largest difference between calculated and measured k_{eff} reached ± 2000 pcm for specific benchmarks. He also showed the difference in k_{eff} due to the $S(\alpha, \beta)$ data provided in ENDF/B-VII.1 and ENDF/B-VIII.0. To conclude, there is an increasing need for ACE temperature data in Korea, including TSL.

2.6. TNSL and URR improvements in FUDGE, C.M. Mattoon (LLNL)

There have been recent improvements in FUDGE and GIDI+. The FUDGE teams wanted to expand the code capabilities to RRR and URR. They are developing new features with GNDS. FUDGE is the main code to maintain, process, and test nuclear data libraries at LLNL. GIDI+ reads the files and does the Monte Carlo sampling of the data from GNDS. All the codes are open source. Recent developments were focused on improving low-energy neutron capabilities, especially for TNSL and URR. GIDI+ allows reading the processed GNDS data. There have been changes in how TNSL data are handled in GNDS (from 1.9 to 2.0). These changes unified the way TNSL data are treated compared to other reaction cross sections. The other advantage is the sampling. Coherent elastic scattering is handled correctly. Currently, they expanded the angular distribution as a function of the incident energy. Recently, they realized that for coherent elastic scattering it would be easier to have GIDI+ sample angles directly from the cumulative structure data (i.e., ENDF-6 $S(E, T)$ data). As far as incoherent elastic scattering is concerned, now they store the data angular distribution as a function of the incident energy. They want to try sampling angles directly from the Debye-Waller integral data $W'(T)$, which are in the GNDS file. C. Mattoon mentioned the new mixed elastic mode (LTHR=3) proposed by M. Zerkle, which is supported by GNDS and FUDGE. Incoherent inelastic scattering is trickier because $S(\alpha, \beta)$ is tabulated as a function of α , and the extrapolation to low and high α does not always work (for forward scattering). They have good results comparing NJOY and FUDGE. The incident energy grid used by NJOY is not always sufficient. FUDGE uses a twice-denser grid. There is a significant difference between NJOY and FUDGE for forward scattering (low α). Processed GNDS can be used with different codes like LLNL's Mercury (MC) and Ardra (deterministic) codes. There are still differences to understand. Is it due to the processing or to the sampling? Concerning URR and self-shielding, it was shown at the previous data processing meeting (IAEA TM on Processing Codes, 23-26 Sept 2019) that FUDGE results differed slightly compared to other codes (see: [Code Validation for Generating ACE Libraries \(iaea.org\)](https://www.iaea.org/publications/CodeValidationforGeneratingACELibraries)). This could be due to the way the cumulative probability distribution

is built. C. Mattoon thinks that there is a bug in both NJOY and FRENDY. To conclude, there is a lot of focus on TNSL and URR regions in FUDGE developments. The TNSL processing is mostly complete, but the sampling code can be improved.

Q&A, comments, discussion:

M. Zerkle: This is a common problem among processing codes (slide 13).

C. Mattoon: We know that there is a bug in the processing code and that we need to refine the grid at low incident energy, but it depends on the load time the user is willing to wait.

Someone: Could you elaborate a bit more on the differences between FUDGE and NJOY?

L. Leal: Do you compute moments or just the mean values?

C. Mattoon: There are different strategies. One is taking cross sections and putting them into a PDF. The traditional method is to sample random points and then derive the probability tables.

K. Tada: I checked the cause of the difference: Do you use equally probable bins?

C. Mattoon: For every URR sample, we do the heating and compute the cross sections for 1000 random points, and at that point, I figure out the bins.

K. Tada: In NJOY and FRENDY in the high cross section range, the probability is very low while in the middle range we use equal probability bins. The bins are adaptive. FRENDY uses 20 probability bins. If we use the same bins, the probability tables are different anyway.

C. Mattoon: In order to generate the plots, I run the code with 50 equal bins. I have to check.

From the chat:

A. Holcomb: Using less approximate cross section formalisms may be computationally prohibitive. Given a sufficient number of bins, the way you bin does not really matter for transport calculations. For example, equiprobable vs non-equiprobable should give statistically equivalent results, given you are using a reasonable number of bins (20 is fine).

K. Tada: In my calculations, I see a difference between equiprobable and non-equiprobable bins in the high and the low cross section region when I use 20 probability bins. I agree that 50 is very fine so the difference is not large.

A. Holcomb: The point of discretization is to approximate the continuous CDF. As long as you have an accurate representation of the CDF, it does not matter which way you bin it. That being said, the choice of binning will affect the variance in each bin. So, it is possible that you are seeing the effect of under-sampling in those bins.

K. Tada: Yes, FRENDY sets the bin using first pseudo resonance structure and the number of sampling is not enough. I should modify the setting method of the bins.

A. Holcomb: Caleb showed that they are saving the values from each realization and then perform the binning at the end. We do the same thing in AMPX-PURM. Perhaps, you could employ a similar method rather than enforcing a bin structure at the start.

J.-Ch. Sublet: Average cross section done by evaluators in MF3 does not warrant consistency with the parameters given in the ENDF file MF2.

A. Holcomb: This was an underlying bug in AMPX when compared to NJOY results. For both LSSF=0/1, the results obtained from sampling the average resonance parameters must be normalized to the average computed directly from the formula before scaling by or adding to file 3.

D. Aldama: Andrew, a question about probability sampling in the URR. As you know, sometimes you get very small values of the scattering cross section due to limitation of the SLBW formalism, the one used in the URR. How do you take care of that in AMPX? NJOY just removes the negative values, but sometimes you get very small values that are not physically expected. In my codes, I limit the minimum value for the total to the $\Sigma_{potential}$ divided by 20.

C. Jeannesson: Wouldn't the most logic approach be to set the elastic cross section to 0 and keep the

total as the sum of the capture and fission? That is NJOY's way of doing things.

D. Aldama: Yes, but sometimes even in this case the value of the total is too small.

A. Holcomb: Because the SLBW elastic cross section can go negative under Doppler broadening, we discard any set of samples that cause a negative broadened elastic cross section. If we sample it negative too many times in a row, we halt execution. For example, we could not process the ENDF/B-7.1 Na-22 cross sections because we were unable to ever sample a positive broadened elastic scattering cross section.

2.7. Treatment of thermal scattering law data in the nuclear data processing code NECP-Atlas, T. Zu (Xi'an Jiaotong University)

The presentation introduces the current status of NECP-Atlas. There are three modules related to the thermal scattering data. Sab_calc module is developed to calculate thermal scattering law (TSL); Therm_calc to calculate scattering cross sections using TSL data; resk_calc to treat the resonance elastic scattering. NECP-Atlas can independently produce the thermal neutron scattering data required in the ACE library.

The multi-point linearization method is developed in NECP-Atlas to refine the incident energy grid of the incoherent inelastic scattering. The refined energy grid can capture more details of the oscillations of the inelastic scattering cross sections, compared with the fixed energy grid. The inelastic scattering data of ZrHx, generated based on the refined energy grid, are used in the calculations of several critical benchmarks. The effect of the incident energy grid on the k_{eff} of the benchmarks is quantified.

In ENDF-6 formatted evaluations, the coherent and incoherent elastic scattering modes are not simultaneously provided for a material. The ENDF-6 format is extended to simultaneously store the TSL data for the two elastic scattering modes, and the ACE format is also extended to store the processed data for the two elastic scattering modes. The effect of using mixed elastic scattering cross sections is analyzed based on the above-mentioned benchmarks.

Q&A, comments, discussion:

A. Trkov: Is the ACE format extension the same that has been proposed by LANL?

T. Zu: Yes.

V. Sinitsa: Did you refine the grid in the same way for all materials?

T. Zu: For graphite and water, the fixed grid is ok. For the ZrH inelastic XS you need a refined grid.

2.8. ACE format development at LANL: Mixed mode thermal scattering and the ACEtk Toolkit, W. Haeck (LANL)

A new ACE format has been proposed to accommodate the mixed mode thermal scattering. When a new ENDF/B library is published, people ask for format changes and addition of data, which require changes in the processing codes as well. ENDF/B-VII.0 and ENDF/B-VII.1 are good examples. In ENDF/B-VII.1 the biggest change was the mixed mode thermal scattering, but also the improved photonuclear data. When the format changes, MCNP must be updated accordingly. Any change must be done together with the MCNP team. It is important that the older versions of the libraries remain usable. For thermal scattering, there are coherent elastic, incoherent elastic, coherent and incoherent inelastic. Before ENDF/B-VIII.0 there were only coherent or incoherent elastic, and the ACE format only allowed for one elastic thermal scattering block. Now, if both are given, an additional block must be added. Coherent elastic is always given first. The modifications will be done in NJOY 2016.65. They include the updates for photonuclear data (done), the update to ERRORR for MF34 covariances using multiple subsections (incomplete), and

other updates for charged particle data. In particular, for the thermal scattering, MODER was modified, and also THERMR (most of the thermal scattering processing happens here). The changes to the ACER module are mostly cosmetic (e.g., plots). For the future, LANL will continue using NJOY2016 for the near future, and will provide support for the new ENDF/B-VIII.1. NJOY21 will shift from module-based to component-based, because the components can be developed and deployed faster than the modules. The components will be developed in C++ and will always have a Python API on top of them. Introducing GNDS to NJOY2016 is impossible because NJOY2016 is very closely linked to ENDF-6. NJOY21 processing components MUST be format agnostic. There are three formatting components: ENDFtk (finished), GNDStk, and ACETk.

Q&A, comments, discussion:

R. Capote: We are discussing how to proceed in the URR with the probability tables. They are enough for self-shielding, but they are linked to the LSSF flag. If LSSF=1, the cross section will be inconsistent with the probability tables. To generate the final probability tables is tricky. Did you consider that your PDF is normalized?

W. Haeck: The resonance parameters are used to generate cross sections for the individual reactions, which are then transformed into probability tables. The average values in MF3 are used in the generation of the probability tables.

A. Trkov: Is there some study on the degree of inconsistency that can be tolerated without making new evaluations?

2.9. URR measurements, evaluation, and testing for Tantalum, Y. Danon (RPI)

See presentation “URR measurements, evaluation and testing for tantalum”, IAEA TM of the International Nuclear Data Evaluation Network (INDEN) on Actinide Evaluations in the Resonance Region (October 21-24, 2019), <https://www-nds.iaea.org/index-meeting-crp/TM-INDEN-2019/>.

Further information will be presented at the upcoming INDEN meeting: IAEA CM of the International Nuclear Data Evaluation Network (INDEN) on Actinide Evaluation in the Resonance Region (November 1-4, 2021), <http://int-nds.iaea.org/index-meeting-crp/CM-INDEN-2021-res/>

In the introduction R. Capote pointed out the importance of this presentation to discuss benchmark for the URR.

Y. Danon presented the motivation for the selection of ^{181}Ta , which is one of the nuclear data needs included in the NCSP list and is a single-isotope element with cross-section fluctuations in the URR which are similar to some actinides. A comparison between JEFF-3.2, ENDF/B-VII.1 and JENDL/4.0 showed significant differences in simulated capture rate for ENDF/B-VII.1 in the URR. He introduced the two URR formats in the evaluated files: LSSF=0 and LSSF=1. Then, processing codes (e.g., NJOY21) generate probability tables for Monte Carlo neutron transport codes (e.g., MCNP6.1). He recommended LSSF=0 because it is self-consistent. He pointed to the “big picture” of using transmission measurements in the evaluation and also the “novel” use of thick target transmission measurements for validating the URR (although it was already done in the past in another context). In his presentation, he commented how the fluctuations enhance transmission which reduces the effective cross section, hence the term self-shielding (for more information see Froehner et al., “Cross-section fluctuations and self-shielding effects in the URR”, NEA-WPEC/SG15, 1995). He showed the results for JEFF-3.3, JENDL-4.0 and ENDF/B-VIII.0 for a thick (12 mm) ^{181}Ta experiment. Experimental uncertainties are 3-5%. He concluded that thick sample transmission experiments are useful for validating URR and URR/RRR boundary.

Q&A, comments, discussion:

R. Capote: complains about LSSF=1, they are not fully consistent because they force the average cross section to be smooth in energy. The LSSF=1 allows some fluctuations in the URR, which are important in some cases.

This discussion should be moved to the evaluators, with potential consequences in the processing, and he suggested to postpone the discussion to the upcoming IAEA CM of the International Nuclear Data Evaluation Network (INDEN) on Actinide Evaluation in the Resonance Region (November 1-4, 2021).

L. Leal: also pointed out that processing should be performed according to the evaluation.

A. Trkov: says that this clean transmission benchmark is useful for validation.

Finally, it was also commented that validation/testing should be independent of evaluation.

2.10. Investigation of some points of methodology in the Unresolved Resonance Range processing, C. Jeannesson (IRSN)

C. Jeannesson presented his PhD work. He introduced the URR parameters, and the probability tables to handle self-shielding. He presented the ladder method, and the comparison of the sampling between NJOY (leftmost resonance first) and AMPX (central spacing first). A methodology to estimate the number of resonances is presented which are required to perform accurate calculations. He pointed out that looking at the $\bar{\Gamma}/\bar{D}$ ratio is a criterion for the number of resonances to consider (a typical minimal required is 100 resonances). For instance, a value of $\bar{\Gamma}/\bar{D} \gg 0.01$ is taken for comparison to handle many resonances with few Monte Carlo iterations. Finally, he described PTs construction and fitting. Usually, 20 bins are considered as a starting point. Different construction methods are compared: linear, equiprobable, NJOY-like and k-clustering. The impact of these methods was compared in different criticality Benchmarks using large equiprobable tables (1000 bins) as reference.

Q&A, comments, discussion:

R. Capote: asked about the impact of LSSF in the processing., Clément clarified that the LSSF option is not used in the resonance sampling based on the URR parameters. The LSSF does not change the methodology, it just adds a contribution to the cross section.

R. Capote: pointed out that both options allow one to calculate the self-shielding, although the self-shielded cross sections predicted from the URR may be an issue.

A. Holcomb: (chat): says that for LSSF=0/1 there is always a renormalization (for LSSF=0 via the cross-section value that can be calculated directly from the average resonance parameters, for LSSF=1 renormalization is via the FILE3 value).

Doro Wiarda (chat): pointed out that if FILE3 has more points than FILE2, it is unclear if extra p-tables should be added for consistency with the interpolation of cross sections (e.g. APMX).

R. Cullen (chat): if the cross section is pre-defined, but there is not a unique pre-defined resonance parameter, additional approximations should be performed. There is not a unique way to do it.

R. Capote: suggested more discussion about the URR evaluation in the upcoming IAEA CM of the International Nuclear Data Evaluation Network (INDEN) on Actinide Evaluation in the Resonance Region (November 1-4, 2021)

A long discussion about fluctuation factors and the interpretation by processing codes followed. Then, L. Leal suggested that processing developers (e.g., Doro, Wim) should work for a better understanding of the interpretation of it.

2.11. Proposal for a benchmark for the validation of the self-shielding treatment in the Unresolved Resonance Region, A. Trkov (IJS)

A. Trkov presented the proposal of a transmission benchmark for a thick tantalum (^{181}Ta) target (12 mm) with measurements at RPI (see: J.M. Brown, et al, Validation of Unresolved Neutron Resonance Parameters Using a Thick-Sample Transmission Measurement, Nucl. Science Engineering 194 (2019) <https://doi.org/10.1080/00295639.2019.1688087>).

A simple model is developed for the simulation of the transmission experiment. A Trkov showed some preliminary results using different codes such as ACEMAKER, TOP (IRSN), TRIPOLI, NNL-ORNL, for both ENDF/B-VIII.0 and JEFF-3.3. He discussed the impact of different RRR/URR evaluations, discontinuity between RRR/URR and extrapolation issues. This example is useful to see how codes deal with highly degenerate cases such as ^{181}Ta resonance evaluation in ENDF/B-VIII.0

Q&A, comments, discussion:

R. Capote/R. Cullen: commented that the problem of the discontinuity between RRR and URR is provoked by a poor evaluation in the RRR. Then, the extrapolation at the discontinuity RRR/URR using GROUPIE is not good.

D. Wiarda (chat): says that AMPX has been changed in the case of additive to normalize the probability table to the infinite diluted values calculated by solving the statistical integral via a method developed by R.N. Hwang at ANL.

(see:https://indico.bnl.gov/event/3580/contributions/10422/attachments/9395/11492/CSEWG_Wiarda_2017_final.pdf). Otherwise, AMPX only uses p-tables for CE and MG.

D. Aldama (chat): says that NJOY uses the same, but NJOY corrects negative values of the scattering cross sections, instead of rejecting these data.

J-Ch. Sublet (chat): also mentioned that URR processing is not unique among processing codes (<https://t2.lanl.gov/nis/publications/200907a.pdf>).

R. Capote: emphasized the importance of processing, especially in the URR. Because URR data in the evaluated files need to be processed for applications.

2.12. Fitting cross-section probability tables, D.A. Brown (BNL)

D. Brown presented Matteo Vorabbi's post-doctoral work. The URR parameters are introduced in a Bayesian approach as probability distributions to measure our ignorance of the cross sections. The resonance ladder methodology implemented in FUDGE is described. Temperature effects are also introduced using two different approaches, the standard (NJOY) and alternate methods. The alternative approach is essentially defined as an event-by-event PDF. A comparison between FUDGE and NJOY shows that an alternative approach has some deficiencies to capture the peak of the capture cross-sections PDF. Then, the alternative method is tested in criticality benchmarks with poor results. This approach is improved using an experimental PDF which gives a strong constraint for the theoretical approach. Finally, D. Brown presented a way to fit the PDFs using regression techniques that may be improved by other ML/IA techniques. The aim is to find a "universal" PDF for each reaction channel. The work is ongoing, with a systematic investigation of the capture channel for all the available nuclei, to be extended to other channels.

He concluded by saying that more benchmark experiments in the URR are needed (see presentation: slide taken from C. Percher CSEWG 2020)

Q&A, comments, discussion:

R. Capote: points out how to derive PDFs related to different channels (e.g. elastic, fission) with self-shielding, not only the total cross section. D. Brown says that correlations between channels exists due to unitarity, so for probability tables one must compute conditional probabilities.

R. Capote: says that there may be different resolution for different channels. Then, constraints based on experiments could be different for different channels. D. Brown comments the possibility of different treatment for different channels to avoid having information in the URR if there is information for the channel in the RRR.

D. Brown and Y. Danon: suggest new methods to avoid smooth cross section for the URR evaluation having measurements with high resolution much closer to reality.

R. Capote: says we need cross sections consistent with measurements which are used in applications, both evaluators and processors should work together.

M. Zerkle: suggests a review of more benchmarks and experiments: For instance, IPPE/Russian – for structural materials for fast reactors in 70s-80s. Other benchmarks are suggested by Y. Danon and L. Leal. In the chat, R. D. Cullen mentions LLNL U5&U8 – Bramblatt and Czirr.

3. Discussion

3.1. Thermal scattering processing

Before the discussion, an overview was given on the results of the intercomparison exercise. It has become clear that the different ACE format options (IFENG=1 or 2, with IFENG=2 being the better format) have a large influence on the results. When IFENG=2 is used, the results for all cases were within 50 pcm from the average result. When IFENG=1 is compared to IFENG=2, the differences between the two can become as large as 300 pcm.

The resulting recommendation is therefore to prefer IFENG=2 for processing thermal scattering files and for processing codes to provide an information message when users process data using other options. As a follow-up exercise, it was decided to reprocess the H in ZrH thermal scattering data using the following characteristics:

- Using the tabulated ACE format (IFENG=2);
- Using 32 angular bins;
- Up to 10 eV;
- Using a tolerance of .3% on the incident energy grid if an adaptive energy grid is used or using a more refined fixed energy grid for processing codes that do not have an adaptive energy grid.

The most important improvement identified in processing concerns the incident energy grid in which an adaptive energy grid algorithm seems to be best to properly capture the oscillating nature of the data.

3.2. Unresolved resonance self-shielding and processing

Through the presentations during this meeting, it has become clear that there are different methods to generate unresolved resonance probability tables.

In order to encourage exchanges between code developers and comparison of codes, it was decided to perform an additional exercise using ^{235}U and Ta evaluations from both ENDF/B-VIII.0 and INDEN evaluations. The comparison will focus on both the probability tables and the underlying distributions as well as the derived average values and self-shielded cross sections that can be derived from the tables.

Exercise specifications are given in Appendix 1.

APPENDIX I: Exercises

EXERCISE-1: TSL Processing verification (Round-2)

Different codes generated ACE-TSL files which gave results for the selected benchmarks showing a spread by up to 100 pcm. The aim of the exercise is to reduce the spread by suitable choice of input parameters. The test case is H in ZrH from ENDF/B-VIII.0 at 296 K (the temperature at which the TSL data are given), as before. The task is:

- Use the formatting option IFENG=2;
- Extend the incident energy range of TSL to 5 eV or 10 eV and check the difference in k_{eff} if applicable;
- Use 32 or more angular bins;
- Use a dense energy grid for the incident neutrons, preferably to ensure reconstruction tolerance of at least 0.3% if an adaptive energy grid is available;
- Compare incoherent inelastic scattering cross section;
- Send the ACE files to the co-ordinator (andrej.trkov@ijs.si).

EXERCISE-2: Self-shielding Verification

Issues were identified in generating probability tables/multi-band parameters that require further investigation. The purpose of the exercise is to compare average unshielded and fully shielded cross sections generated by different codes on a coarse energy grid in energy groups just below and just above the RRR/URR boundary (and just below and above the URR/fast boundary). Specifications for the exercise are:

- Process two evaluated data files for U-235, namely one from the ENDF/B-VIII.0 library and the INDEN file “u235ib46o28t6DNcnu5ef0STzt” available from <https://www-nds.iaea.org/INDEN/> (see the U-235 tab);
- Process two ^{181}Ta evaluated data files, namely one from the ENDF/B-VIII.0 library and the other from JEFF-3.3, which are available from the IAEA web site;
- Process the total, elastic, capture (and fission, if applicable) cross sections at 293.6 K;
- Use the energy-group structure as used in Standards-2017 given below;
- Use the 1/E weighting spectrum in the resonance range;
- Include background cross sections for self-shielding that correspond to infinite dilution and full shielding (as close as possible). Intermediate values can also be specified, if desired, for example: “1.e-10, 1000000.0, 100000.0, 10000.0, 1000.0, 100.0, 10.0, 1.0, 1.e-3, 1.0E-6”;
- Send the results of calculations to the coordinator (A. Trkov). The format can be a two-column format for the cross sections, the full NJOY group format (GENDF) or the ACE format (if you cannot produce the group data, in which case group-averaging will be done by the coordinator).

Note: The relevant groups for ^{181}Ta from ENDF/B-VIII.0, for example, are groups 13 and 15, but the full energy group system can be used, if desired.

The energy-group structure [eV] of IAEA Standard 2017:

1.0000E-05	5.6000E-01	7.8000E+00	1.1000E+01	2.0000E+02	3.0000E+02
4.0000E+02	5.0000E+02	6.0000E+02	7.0000E+02	8.0000E+02	9.0000E+02
1.2250E+03	2.0000E+03	3.0000E+03	4.0000E+03	5.0000E+03	6.0000E+03
7.0000E+03	8.0000E+03	9.0000E+03	1.2250E+04	1.7500E+04	2.2000E+04
2.7000E+04	3.7500E+04	5.0000E+04	6.0000E+04	7.0000E+04	8.0000E+04
9.0000E+04	9.7500E+04	1.1000E+05	1.3500E+05	1.6000E+05	1.7500E+05
1.8500E+05	1.9500E+05	2.0500E+05	2.1500E+05	2.2500E+05	2.3250E+05
2.3750E+05	2.4250E+05	2.4750E+05	2.5500E+05	2.6500E+05	2.7500E+05
2.9000E+05	3.1250E+05	3.3750E+05	3.6250E+05	3.8750E+05	4.1250E+05
4.3750E+05	4.6250E+05	4.8750E+05	5.1000E+05	5.3000E+05	5.5500E+05
5.8500E+05	6.2500E+05	6.7500E+05	7.2500E+05	7.7500E+05	8.2500E+05
8.7500E+05	9.2000E+05	9.5000E+05	9.7000E+05	9.9000E+05	1.0500E+06
1.1750E+06	1.3250E+06	1.5000E+06	1.7000E+06	1.9000E+06	2.1000E+06
2.3000E+06	2.5000E+06	2.7000E+06	2.9000E+06	3.3000E+06	3.8000E+06
4.2500E+06	4.6000E+06	4.8500E+06	5.1500E+06	5.4000E+06	5.6500E+06
5.9000E+06	6.1000E+06	6.3500E+06	6.7500E+06	7.2500E+06	7.6250E+06
7.8750E+06	8.2500E+06	8.7500E+06	9.5000E+06	1.0500E+07	1.1250E+07
1.1750E+07	1.2500E+07	1.3500E+07	1.4250E+07	1.4750E+07	1.5500E+07
1.6500E+07	1.7500E+07	1.8500E+07	1.9500E+07	2.0500E+07	2.1500E+07
2.2500E+07	2.3500E+07	2.4500E+07	2.5500E+07	2.6500E+07	2.7500E+07
2.8500E+07	2.9500E+07	3.1000E+07			

APPENDIX II: Adopted Agenda

Monday 18 October (starting 2pm, open 1:45pm Vienna time)

2:00 – 2:05	Opening of the meeting
2:05 – 2:15	Election of Chair and Rapporteur(s), discussion of Agenda
2:15	Welcome, Andrej Trkov (IJS, Slovenia)
	Andrej Trkov: "Current achievements of the code verification project for generating ACE libraries"
<i>Short break</i>	
	Daniel L. Aldama: "Processing thermal scattering law and dosimetry files for Monte Carlo calculations using ACEMAKER"
	Kenichi Tada (JAEA): "Treatment of thermal scattering law data in FRENDY"
	Valentin Sinita "Capabilities of the GRUCON code package in the TSL data processing"

Tuesday 19 October (starting 2pm, open 1:45pm Vienna time)

2:00	Do Heon Kim: "TSL Data Processing for MCNP in KAERI"
	Caleb Matoon: "TNSL and URR improvements in FUDGE"
	Andrej Trkov: "Validation of codes for generating thermal scattering libraries in ACE format"
	Wim Haeck: "ACE format development at LANL: mixed mode thermal scattering and the ACEtk toolkit"

Wednesday 20 October (starting 2pm, open 1:45pm Vienna time)

2:00	Andrej Trkov: "Proposal for the validation of self-shielding methods in the unresolved resonance range"
	Clément Jeannesson: Title to be provided
	Dave Brown: "Fitting the cross-section probability tables"
	Discussion on the self-shielding benchmark

Thursday 21 October (starting 2pm, open 1:45pm Vienna time)

2:00	Discussion on ACE data processing
	Initial Drafting of the Meeting Summary report

Friday 22 October (starting 2pm, open 1:45pm Vienna time)

2:00	Discussion and review of the Meeting Summary report
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APPENDIX III: Participants

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APPENDIX IV: Presentation Links

#	Author	Title	Link
1	A. Trkov	Current Achievements of the Code Verification Project for Generating ACE Libraries	PDF
2	A.Trkov	Comparison of results for ICSBEP benchmarks containing ZrH using TSL libraries for H in ZrH processed by different codes	PDF
3	D. Lopez Aldama	Processing thermal scattering law and dosimetry files for Monte Carlo calculations using ACEMAKER	PDF
4	K. Tada	Treatment of thermal scattering law data in FRENDY	PDF
5	V. Sinitsa	Capabilities of the GRUCON code package in the TSL data processing	PDF
6	D.H. Kim	TSL Data Processing for MCNP in KAERI	PDF
7	D. Brown, et al.	Fitting the cross-section probability tables	PDF
8	C.M. Mattoon	TNSL and URR improvements in FUDGE	PDF
9	Tiejun Zu	Treatment of thermal scattering law data in the nuclear data processing code NECP Atlas	PDF
10	Y. Danon	URR measurements, evaluation, and testing for tantalum	PDF
11	C. Jeannesson	Investigation of some Points of Methodology in the Unresolved Resonance Range Processing	PDF

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