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Nuclear Data Processing

Summary Report of the Technical Meeting
IAEA Headquarters, 3-6 September 2018

Prepared by

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1. Introduction

Part of this meeting is to report on Stage 1 of the ACE verification project (U–235 and U–238 without probability tables). This first stage was discussed at the meeting in December 2017 (see Report INDC(NDS)-0748). The ENDF files to be processed are from ENDF/B-VIII.beta4. The remaining files used for the criticality calculations are the data files that were processed with NJOY at Los Alamos National Laboratory from ENDF/B-VII.1 and distributed with MCNP 6.1. (LA-UR-13-20137, LA-UR-13-20240).

Prior to the meeting, participants submitted ACE files processed with their respective codes. Trkov compared the cross sections in the ACE files to the reference cross sections as processed by PREPRO (IAEA-NDS-39 Rev. 18). PREPRO was chosen as the reference processing code because it is considered robust and reliable.

To test the ACE files submitted by participants, 32 critical benchmarks from the ICSBEP Handbook were used and the k_{eff} values calculated. The list of benchmarks is available on the Project web page https://www-nds.iaea.org/ACE_verification/. Monte Carlo k_{eff} calculations were performed with MCNP 6.1 using the same input decks and the U-235 and U-238 ACE files generated and submitted by the participants. The ACE files generated by NJOY--- and the k_{eff} values calculated by MCNP with those ACE files---were arbitrarily chosen as the reference values; the remaining calculations were compared to the reference calculations. The comparison of the generated ACE files and the results of the critical benchmark calculations constitutes Stage 1 of the study. The results of the 1st stage of this study can be found here: https://www-nds.iaea.org/ACE_verification

2. Presentations by Participants

2.1. Verification of GRUCON Modules and Calculation Procedures for ACE File Generating, V. Sinitsa

- There is a module of GRUCON that produces the ACE file called (naturally) GRUCON/ACE
- GRUCON changed the hard-coded upper limit of the neutron energy range from 20 MeV and now uses an input option to define the upper limit. 30 MeV was used for U–238 and U-235
- Doppler broadening is applied to all cross sections, not just to those with reconstructed resonances
- The results were compared with what was processed with PREPRO; the differences were consistent with the resonance reconstruction tolerance
- The difference in the k_{eff} values as calculated using the critical benchmarks were mostly within 20 pcm, when self-shielding was not included.
- When including probability tables, there were several benchmarks that were 500 pcm different from those calculated by NJOY.
- A difference between what is produced in GASPR (hydrogen and helium production) in NJOY and ACER was reported and needs to be checked. (See comments Kahler and Haeck below.)

- o Kahler found an issue in GASPR that LANL will correct in a future version of NJOY2016.
- New functionality of GRUCON:
  - o Revision of GRUCON to handle new ENDF/B-VIII.0 data formats.
  - o There is a question about how to use the new data in the ACE files. Kahler mentioned that we are waiting to see what the MCNP team is going to do about it.
  - o There is a new Doppler broadening scheme to smooth out the Legendre polynomial coefficients reconstructed from the resolved resonance parameters
- Processing of GNDS data in GRUCON/GNDS:
  - o Translation of GNDS files to GRUCON Standard Structures
  - o A number of input parameters are required to do this; everything is pretty similar to what is already required for data processing
  - o A comparison of the GNDS processed data with the ENDF processed data — for the resolved resonance parameters. There are many differences, but the difference appears to be < 1%; within the resonance reconstruction tolerance of the calculation. Sinitsa feels that the difference was not due to the processing, but because of the code that does the comparison. There is a difference in the number of digits written for the reconstructed cross sections to the GNDS file between GRUCON/GNDS and FUDGE.
- In short, GRUCON can process ACE files with little difference when compared to NJOY.
- Sinitsa said he used NJOY2016 (from about two months ago)

Questions
- **Kahler** mentioned that nobody has changed the GASPR in quite some time and so was concerned about the differences reported.
  - o **Haeck** and **Kahler** did a quick investigation and found no differences between what was reported by GASPR and what is in the ACE file using NJOY2016.26.
- **Tada** said he also compared to NJOY and found no differences, although Tada said he is using NJOY99.
- **Trkov** suggested that Sinitsa describe how he compared the gas production so that others can also perform the same calculation and make the same comparisons.
- **Sinitsa** said the biggest difference in the gas production came from processing B-10.
- **Beck** asked how many points were created during the resonance reconstruction.
  - o For U-238, GRUCON produces about 930,000 points in united energy greed for all reactions; FUDGE produces about 440,000 points for total and about 1,000,000 points for radiative cross section.
- **Kahler** and **Haeck** checked the NJOY source code and found that there is indeed double counting in NJOY when partial (discrete level) data exist for charged particle emission (MT600-850) but the summed contribution are not present (MT103-107).

2.2. ACEMAKER: Treatment of self-shielding and new functionalities, *D. Lopéz Aldama*

- IAEA is supporting the production of ACEMAKER to create ACE files.
- ACEMAKER is a package that uses PREPRO, URRFIT and a series of other codes.
- The purpose of the ACEMAKER code package is to generate continuous-energy fast neutron ACE files.
- URR-PACK is a code to calculate self-shielding and is based on three papers by Dermot "Red" Cullen and Andrej Trkov.
- ACEMAKER itself is composed of other components:
    - GETURR
    - URRFIT
    - SIXLIN
    - DOACE
- The self-shielding calculation is done using the multi-band method.
- Photon production processing has been added to ACEMAKER and is currently being verified.

Questions/Comments
- **Sinitsa**: What is the approximation error of the two-band method? This will be investigated in the next stage.
- **Conlin**: Why NJOY2012 was used instead of NJOY2016? NJOY2016 gives the same results; NJOY2012 was used because that was what was available.
    - Many of the changes in PURR would not affect the comparison.
- **Kahler** brought up that there are some evaluations in ENDF/B that have unresolved resonance parameters, but no resonance parameters. ACEMAKER needs to be checked to see what happens in these cases.
- **Tada** wanted to know how to use the multi-band method and how to put the data in the ACE file. Please refer to the IAEA report INDC(NDS)-0711.

2.3. Improvement of probability table generation using ladder method, *K. Tada*

- Tada is the author of the FRENDY processing code and reported on the improvement of the ladder method for the unresolved resonance region
- FRENDY is a JAEA code, begun in 2013.
- Goal is to generate continuous energy cross section library for Monte Carlo codes.
- FRENDY is similar to NJOY99.
- FRENDY will be released in 2019 and will be able to process the ACE library. FRENDY will be released internally in Japan, but will also be made available at the NEA Databank.
- Treatment of unresolved resonance region:
    - Generated by the commonly used "ladder method"
- Improvement of ladder method is done by:
    - Calculation of complex error function:
        - Used in the calculation of the SLBW resonance parameters using the psi-chi method

- Complex error function cannot be calculated exactly, but can be approximated using the 4-pole Padé function.
  - Improvement of chi-squared random numbers
    - NJOY99 uses discrete random numbers.
    - FRENDY uses continuous random numbers.
    - FRENDY's random numbers are a better match to the chi-squared distribution for mean, variance, skewness, and kurtosis than the random numbers generated by NJOY99.
- The results were compared to those of NJOY99 as calculated using BROADR and SIGMA1 modules using JENDL–3.3
- A figure was shown in the Th–229 cross section from JENDL–3.3. The results between FRENDY and NJOY99 are mostly the same. There is a relative difference up to 1.0% in some regions. The high precision method is not required to match with NJOY99.
- FRENDY's probability table is not very different to what is calculated by NJOY99, but is about 20% faster.
- It was determined that 100 ladders are enough to reduce the tolerance to 0.1%.
- When comparing the benchmark calculations, there is a difference of about 0.06% or 60 pcm at most. Not all of the 32 benchmarks were performed by Tada, in fact, the benchmarks that were calculated are different from the suite of 32 tests from Trkov. The ones reported are the ones from the Mosteller suite that had the largest difference.
- FRENDY version 2 is anticipated in 2021 and will include multi-group library and covariance processing.

Questions:
- **Kahler** asked if Monte Carlo benchmark calculations were also compared when using only 10 ladders. (What was reported was when using 100 ladders.) Tada felt that using smaller number of ladders does not have a large impact on the end result.
- **Kahler** mentioned that anything in the unresolved resonance region is absolutely wrong in detail, but on average is correct. Tada has simply demonstrated another way of averaging the data.

2.4. Current Status on the Galilee-I code, *C. Jouanne*

- The first set of ACE files were sent to Trkov who made some comments.
- Improvements were made to Galilee–1 to fix various issues pointed out by Trkov. New files seem to do better.
- When comparing Galilee–1 to PREPRO15 with the old files, there is a difference ($>8\%$) in the energies near threshold. The improved data files show little difference from what is calculated with PREPRO.
- Criticality benchmarks were re-analyzed. Simulations were also performed using TRIPOLI-4. Comparison was made with NJOY2016 and CALENDF.
  - The large discrepancy is due to the processing methods; CALENDF relies on the total cross section in the evaluation file while NJOY2016 recalculates the total cross section from the partials.

- There is a problem in ENDF/B-VIII.0 Pu–239 where the sum of the partial cross sections does not equal the total. This is a known problem.
- With a modified evaluated file, good agreement is seen between MCNP and TRIPOLI-4.

- An analysis was performed to sample the unresolved resonance range. The CDF was calculated from GTREND and PURR and found that there was a somewhat important difference.
- It is planned to provide probability tables using GTREND; group-wise and point-wise (for MCNP).

Questions/Comments
- **Sublet** questioned whether there was a calculation of point-wise data from group-wise data. At first, Jouanne just performed a translation.
- **Trkov** said that Red Cullen had asked that an effort should be made to enforce consistency in data files in the redundant cross sections (i.e., summations) before they are released in ENDF/B. Trkov asked whether this was being heeded. Brown stated that there is automated testing of all of the files, but viewing the results requires human intervention which was neglected due to this happening late in the process.
- **Trkov** asked what the time scale was for implementing probability tables in Galilee–1. Perhaps one year was the answer.
- **Haeck,** with respect to the inconsistency between the total and partial cross sections, NJOY2016 now reports that there is an inconsistency and warns the data processor when running PURR to check the evaluation.

2.5. Progress on ACE file processing by RULER, *P. Liu*

- RULER can do direct Doppler broadening of ACE files after the 0 Kelvin version has been created
- Trkov analyzed the ACE files produced in the first iteration and found the Doppler broadening results were incorrect when multiple temperatures are processed at the same time. Now, only one temperature is processed at a time.
- The double-differential cross sections produced by RULER are being checked
- Should the ACE files produced by RULER include probability tables?
  - There are a limited number of people working on RULER
  - RULER is still under development
  - What method should be used to generate the probability tables? Ladder sampling or multi-band? This depends on the code designer.
- Should ACE files produced by RULER include photon-production data? In principle, yes.

Questions
- **Trkov**: how is the ACE file assembled from the different components?
  - We can Doppler broaden from a given 0 Kelvin ACE file.
  - Their resonance reconstruction data is written directly as an ACE file.

2.6. Processing GNDS for Monte Carlo and Multi-group Transport Codes, B. Beck

- FUDGE is their processing code; all formats must be translated first to GNDS (or ENDL) for processing.
- GIDI/MCGIDI is the API for their (deterministic/Monte Carlo) transport codes for handling GNDS data.
- LLNL has a V&V suite for benchmarking the data
- GNDS stands for — Generalized Nuclear Database Structure
- Several pieces of the GNDS documentation are coming from Subgroup 38 of WPEC.
- Two new subgroups have been formed by WPEC:
    - EG-GNDS: Expert Group on GNDS which is a long-term sub-group tasked with maintenance of GNDS
    - Subgroup 43 in WPEC tasked with development of API/implementation for working with GNDS-formatted data
- GNDS should be considered as a way to share data. It may not be optimal for use directly in a transport code.
- There are still a few issues that need to be resolved regarding GNDS:
    - Thermal scattering law
    - Fission fragments/delayed neutrons
    - Decay data
    - Updates to handle the new ENDF–6 fission formats introduced for ENDF/B-VIII.0
    - Currently there is no way to put into ACE the probability tables using FUDGE
    - Is GNDS flexible enough to handle experimental data (e.g., exfor, ENSDF)?
- One should expect minor changes to GNDS over the next few years as it becomes more widely adopted.
- If we could put experimental data into GNDS, FUDGE can read it.
- FUDGE — For Updating Data and Generating Evaluations includes several features:
    - Many different capabilities with more coming all the time
    - Available from https://ndclx4.bn.gov/gf/project/gnd
    - Hope to have unresolved resonance probability tables by next release (November 2018?)
    - The need to develop thermal scattering data remains
- FUDGE can create an ACE file without probability tables (with toACE.py) from a GNDS file
- Livermore has two APIs for accessing GNDS-formatted data:
    - GIDI: For reading in a GNDS file. It has complete support needed for deterministic codes
    - MCGIDI: uses GIDI to read in GNDS data and then puts it into a form more suitable for Monte Carlo transport. Also provides sampling functions
    - It is intended to release GIDI and MCGIDI *soon* under BSD license
    - Both APIs have many capabilities

- Both ENDF/B-VII.1 and ENDF/B-VIII.0 were translated and processed with FUDGE
- V&V suite was designed to test the data, but implicitly also checks the data processing — because one has to process the data before they can be checked.
- Some k_{eff} calculations have been performed. When compared against MCNP calculations, they are similar.
- Starting to do extensive testing by using MCNP to compare FUDGE generated ACE files to NJOY generated ACE files.
- It is intended to release a new version of FUDGE for Python 3.6+. In addition, there will be many other upgrades

Questions/Comments
- **Sublet**: Why do you want to store so much data when you can Doppler broaden on the fly?
    o We don't have the ability to Doppler broaden on the fly and neither does anyone else.
- **Sublet**: Should you store the 0 K data?
    o You should always store the 0 K data as it is needed for some Monte Carlo calculations.
- **Sublet**: I would like to have the data libraries with the resonances reconstructed distributed along with the resonance parameters.
    o When translating a file from ENDF-6 to GNDS, FUDGE will do this if requested.
- **Tada**: We would like to have other experimental data put into GNDS as well.
- **Trkov**: There is more than 50 years of experimental data in EXFOR. Is it worth converting this to the GNDS format?
- **Sublet**: Does GIDI really handle the recoil matrices?
    o Historically we handle several light-ion particles. If the data are there, we can handle them.
    o GNDS/FUDGE/GIDI handles all incident/outgoing particles in the same way. It relies upon the evaluated data being complete.

2.7. NJOY Status in 2018, *J. Conlin*

- NJOY2016 is freely available with Open Source license
    o It can be obtained from https://github.com/njoy/NJOY2016
    o One must use NJOY2016.26 or a later version to properly process ENDF/B-VIII.0. W. Haeck is continually working on fixing bugs.
- NJOY2016 is formally deprecated
    o Only bug fixes will be added to NJOY2016. Bug fixes will only be made for a few more years.
    o All users are encouraged to move to NJOY21 for their production needs
- NJOY21 is the current production version of NJOY2016
    o It can be obtained from https://github.com/njoy/NJOY21
    o It is released with Open Source license like NJOY2016

- - Extensive input verification is performed helping to ensure that your input deck is valid. Note: input verification *cannot* ensure that your input is correct; it can only ensure that it is valid.
- Resonance reconstruction implementation for NJOY21
  - It can handle SLBW, MLBW, Reich-Moore, and R-Matrix Limited (coming later in 2018).
  - Reconstruction results in the same cross-section values as for NJOY2016
    - Within the limitations of the SIGFIG subroutine
  - Reconstruction is up to 8 times faster---particularly for the long-running reconstruction problems (i.e., U-238)
  - It is independent of where the data comes from e.g., ENDF or GNDS
- ACE format specification is now available
  - One can find it at https://github.com/nucleardat/ACEFormat
  - Currently only the incident neutron specification is supported. Others will follow, including continuous TSL representation.
  - If problems are found, please submit an issue on github.com
- Any questions or concerns about NJOY2016 or NJOY21, please email njoy@lanl.gov

Questions/Comments
- Are you considering changing the input format for the future?
  - Yes. Likely to use something like a JSON
- How does someone know exactly what version of NJOY they are using?
  - We need to create something like this.

2.8. Benchmark Calculations for U–235 and U–238 Multi-Band Data Based on ENDF/B-VII.1 and ENDF/B-VIII.0b4, D.H. Kim

Multi-band data processing:

- URR-PACK consists of two major modules, URRDO and URRFIT, to produce multi-band data for the unresolved resonance self-shielding treatment. URRDO can calculate multi-band probability tables from the NJOY-generated probability tables and URRFIT can calculate them from the original evaluated data.
- The resulting 2-band probability tables from URRDO and URRFIT for U-235 and U-238 total cross sections were compared with the NJOY 20-ladder probability table. Both 2-band probability tables showed slightly different probability bin boundaries for U-235 and U-238. The probability tables from ENDF/B-VII.1 and ENDF/B-VIII.0b4 showed similar tendencies but slightly larger differences for the 20-ladder and 2-band data originating from NJOY PTM.

Criticality benchmark calculation results

- The criticality benchmark calculations for 32 benchmarks have been carried out with three types of probability tables as well as the one turning off PTABLE from 20-ladder probability table.

- The C/E results with probability tables showed good agreements each other, but they showed large discrepancies for some IMF (e.g., BIG-TEN and ZPR-6/9) and MIF benchmarks when compared to the C/E results without probability tables. The discrepancies tend to be reduced for ENDF/B-VIII.0b4 compared to ENDF/B-VII.1.
- The k_{eff} ratios by ENDF/B-VII.1 can reproduce the work reported in INDC(NDS)-0711 by D.E. Cullen well. Large self-shielding effects for some IMF and MIF benchmarks were observed due to U-235 and U-238 cross sections. For ENDF/B-VII.1, the results with the 2-band probability table from URRFIT showed differences larger than 0.1% for 3 BFS benchmarks compared to those with the 20-ladder probability table. For ENDF/B-VIII.0b4, all the 2-band results agreed well within 0.1%. Without unresolved resonance self-shielding, k_{eff} ratio differences between ENDF/B-VII.1 and ENDF/B-VIII.0b4 were up to ~0.1%.

Questions/Comments
- **Trkov**: Seemed to remember smaller differences in a different publication.

2.9. Current status of the GAIA processing code, R. Ichou

- GAIA-1 is designed to minimize the effort of generating nuclear data libraries (NJOY wrapper)
- Currently uses NJOY2016.35
- It produces ACE, PENDF, XML, and GENDF formatted files.
- It is the current tool for nuclear data library generation at IRSN
- GAIA-2 is under development, independent of NJOY.
    - Stand-alone C++ modular processing code project
    - Resonance reconstruction and Doppler broadening in a single step. This has already been implemented.
    - Read from ENDF and GNDS
    - It can be used as a stand-alone application or integrated into other applications
    - Improved formalism for covariance generation
    - Improved formalism in the unresolved resonance range
- In good agreement with PREPRO, but the data has some issues with the criticality benchmarks that were used in this study
- Generalized R-Matrix
    - Result of Ghislain Ferran's PhD thesis
    - Using R-matrix S-T decomposition
- GAIA integrates the Doppler broadening with the resonance reconstruction by utilizing fast Fourier transforms. Another option is based on the solution of the heat equation. This has some limitations in the resonance region.
- Working on a new H_2O thermal scattering data which could be fed into NJOYs LEAPR module, but can also be directly generated without NJOY. Based on new experiments by Vaibhav Jaiswal PhD thesis and molecular dynamics simulations.
- Unresolved resonance region processing
    - Based on Clement Jeannesson PhD thesis

- o Will be implemented in the TOP module
- o Working towards an analytical representation instead of probability tables
- Want to be independent of NJOY

Questions/Comments
- **Trkov**: Do you have more flexibility in the boundary conditions with Generalized R-Matrix formalism?
  - o We use whatever SAMMY has.
- **Trkov**: What is the time scale of the development of the unresolved resonance treatment, heating, etc.?
  - o Unresolved resolved range was begun one year ago, expecting something in two more years.
  - o Heating is planned, but no specific timeline right now.
- **Sublet**: Codes other than NJOY can do the heating. Other fields (e.g., high energy physics) do this all the time. They typically do this with event generators.
  - o For low energy applications, you must still use a processing code (NJOY is practically the only one that can do it) and tabulated data.
- **Kahler**: Have you compared your new Doppler broadening scheme with the existing methods?
  - o Cross-section results compared nicely for reactor-like temperatures.
- **Sublet**: Does the option to Doppler broaden threshold reactions still exist in NJOY?
  - o Yes. We have not taken anything out. It's just a result of the mathematics. However, we have to remove the non-zero cross sections below the Q-value to keep the transport codes happy.

2.10. Serpent and evaluated nuclear/atomic data, *V. Valtavirta*

- http://montecarlo.vtt.fi
- http://serpent.vtt.fi
- Development of Serpent was begun in 2004; desire to have a simplified Monte Carlo transport code for reactor physics
- Serpent applications has expanded since then
- Serpent has been outgrowing the ACE format with new applications requiring data not supported by the ACE format (because it isn't supported by MCNP) and the fact that the ACE format specifications are not publicly available.
- Some new ACE files don't go through the reading routines and there is the assumption that the format is changing.
- Finland is still very interested in nuclear reactor simulations
- A new reactor calculation framework, "Kraken", is under development
- The intention is to build expertise in young people and develop source-code level knowledge
- Leverage the existing tools while beginning the development of new tools
- Applications include:
  - o Group constant generation
  - o Multi-physics calculations
  - o Radiation transport

- o Fusion neutronics
  - o Radiation shielding, medical applications
  - o Sensitivity and uncertainty applications
- Much needs to be done that requires nuclear data
- Serpent capabilities:
  - o Multi-purpose 3-D Monte Carlo transport code
  - o Burnup
  - o Automatic generation of group constants
  - o Coupled multi-physics calculations
- Neutron physics:
  - o Still read cross sections from ACE files
  - o Use probability tables for unresolved resonance range
  - o Use S(alpha, beta) data for thermal scattering
  - o On-the-fly temperature treatment for continuous energy cross sections and S(alpha, beta) kernels
  - o Nuclear data used in Serpent is processed with NJOY
- Photon physics:
  - o Previously used ACE-formatted data
  - o Photoatomic interactions
  - o Atomic relaxation and thick-target bremsstrahlung approximation included
  - o Many data requirements taken from ENDF and many other sources
  - o Used to use data from ACE files
  - o NJOY lacks support for some photo atomic data
  - o No documentation on the new "eprdata" library format of MCNP
  - o Will generate own data using JSON-format
  - o Libraries are based on ENDF/B-VII.1 and EPICS2017
- Energy deposition calculations
  - o Most accurate method uses coupled neutron-photon transport in Serpent 2
  - o Mode 0: All energy is deposited locally at fission site
  - o Mode 1: Local energy deposition based on ENDF MF 1, MT 458 data
  - o Mode 2: Local photon energy deposition with neutrons depositing their energy along their history in various locations
  - o Mode 3: Coupled neutron-photon transport. Neutrons and photons deposit their energy along transport history.
  - o Modes 1—3 require data that is not available in ACE format
  - o Data is currently appended to the ACE file in a post-processing step
- Uncertainty propagation
  - o Based on collision history
  - o Several applications
  - o Can be done by post-processing, but would be better to do it internally
  - o Currently read COVRX (binary and ASCII) and will implement reading of Boxer format soon.
  - o Could use continuous-energy covariance data instead of multi-group data if available.
- Would like to know how to specify isomeric state in the ACE file
- Energy dependent branching ratios and needed for improved burnup calculations

- Need energy dependent mean scattering cosines to reduce workload on Serpent

- **Trkov**: What was the problem with EPICS2017?
  - Atomic relaxation problems
  - There was a recent update to EPICS2017 that may have fixed the problem
- **Brown**: There are three sources of EPICS2017 that don't agree with each other. There are serious issues with all three sources of data.
- **Sublet**: I've always added energy deposition data in ACE. It may not be officially supported, but it can be done.
- **Conlin**: I have tried to figure out the continuous-energy S(alpha, beta) format, but it has not been formally published.
- **Haeck**: Photoatomic data libraries are not processed by NJOY, but by some other code developed by the MCNP team. This code is being integrated into ACEtk for NJOY21.

2.11. Resonance QA, *D. Brown*

- Brookhaven doesn't own any processing code, but uses all of them while testing ENDF files.
- Testing is automated with the ADVANCE continuous integration system
- Cumulative level distribution already tells us a lot. It's a simple check, but we can do better than that
- We can tell, for example, if levels are missing based on the shape of the distribution of spacing of levels
- There are several metrics that can be used to quantify the density/spacing of resonances/levels that can help us to identify if some are missing.
- Stochastic Resonance Generation
  - Fake resonances have many uses
- It is intended to put statistical resonance generation into FUDGE using mcres.py

Questions/Comments
- **Conlin**: What is the website for the ADVANCE server?
  - http://www.nndc.bnl.gov/endf/b7.dev/qa/index.html
- **Haeck**: Do you have documentation?
  - It's coming
- **Morgan**: How confident are you in your assumptions?
  - The scientific community consensus is that random matrix theory is "good enough".
- **Koning**: Are you going to fill in the resonance region for the future of ENDF/B
  - There are many who are nervous about artificial resonances in ENDF/B
- ENDF does not have a mechanism to distinguish artificial or manufactured resonances from fitted resonances, but GNDS could (should?) be modified to allow this. This could pose some problems to the "poor user" who isn't familiar with the intricacies of the different kinds of resonances.

2.12. Results of ACE Library Code Verification Project — Stage 1, *A. Trkov*

- The motivation for this was to have an option other than NJOY to generate application libraries. Some member countries could not get NJOY because of its restrictions. Also, there is a need for more than one processing code.
- ACE stands for A Compact ENDF and is used for many Monte Carlo codes
- Stage 1:
  - Objective: verify that codes can assemble the cross sections correctly into an ACE file
  - Statistics: many variants of ACE file assembly with more on the way
  - Participating Codes:
    1. NJOY2016/NJOY21
    2. LEGEND/NJOY2012
    3. PREPRO/ACEMAKER
    4. FRENDY
    5. FUDGE
    6. GAIA/NJOY2016
    7. GALILEE-1/NJOY2016
    8. GRUCON
    9. NECP-Atlas
    10. RULER
    11. AMPX
  - Procedures
    - Test cases U–235 and U–238 from ENDF/B-VIII.0 b4
    - Cross-section comparison to PREPRO, including angular distributions and double-differential data using modules of PREPRO, ENDVER and auxiliary codes. PREPRO was chosen because it is very robust and stable.
  - Generally, all codes agree with respect to cross-section reconstruction.
  - It appears that many of the differences occur at the boundaries of resonance and unresolved resonance regions. Each code has a different way of dealing with boundary discontinuities. Such differences are physically insignificant.
  - Trkov took the different ACE files and ran the suite of 32 benchmarks in MCNP. In most cases, the difference between the reference (NJOY) and the other code was < 20 pcm. There are a few that fall outside the range, but all are < 60 pcm.
  - Conclusion: Stage 1 successfully completed
- Stage 2 will involve calculations with self-shielding/probability tables
- Additional stages to be determined:
  - Photon production
  - thermal scattering
  - Heating/damage …
  - Charged particles

- **Trkov**: What should be the next stage?
  - There seemed to be a fair amount of discussion about the photon production
- **Sublet**: How are you going to test/compare the self-shielding of the generated ACE files.
- **Tada**: Photon production implementation is not high on our priority list. We can't promise that we will be able to do this anytime soon.
- **Conlin**: When are Stage 2/3+ expected to be done?
  - Stage 2 can be done this year because Trkov already has the data files from the participants
  - Other stages will be done sometime in the future

2.13. Current State of AMPX, *D. Wiarda*

- AMPX is mature and robust, thus, consisting of many different modules
- Many of the modules have been modernized and no longer need to write "scratch" files to communicate between modules
- Can process to both continuous-energy (for KENO, Shift), multi-group-energy, covariance, and decay libraries
- Can use a GUI to facilitate the use of AMPX. Given a few parameters only; AMPX will fill in the rest from built-in templates.
- Moving data to HDF5 format as the final continuous-energy library
- All data is converted to in-memory resource for processing and Monte Carlo transport
- The SCALE module Fulcrum can be used to plot data from all the different data files
- Only a small number of the AMPX modules read/write ENDF, and even those just use a specific subroutine.
- When GNDS comes along (some of it can already be done) it will be easy to process the data as the routines themselves are independent of the source of the data. Complete GNDS processing for incident neutrons is expected to be available in the next SCALE 6.3 beta release.
- Have processed ENDF/B-VIII.0 to both continuous-energy and multi-group-energy. This data will be released with SCALE 6.3 beta, later in 2018 or early 2019.
- AMPX requires a patch to process ENDF/B-VIII.0 due to the new formats. Send email to Doro Wiarda to get that patch.

Questions/Comments

- **Haeck**: Does the HDF5 data use GNDS?
  - No. It is optimized for the Shift Monte Carlo code (part of SCALE)

2.14. Updating NJOY's HEATR module for ENDF/B-VIII.0, *W. Haeck*

- A number of reports have been written describing the NJOY reports that have been made in NJOY2016. If you want to get the document (LA-UR–18–22676) search for the number at http://www.osti.gov

- The ENDF format is often changed/updated with the release of a new ENDF/B library. These changes require modifications to processing codes.
- NJOY modules have been updated to either use or ignore the new formats
- One of these changes was the fission energy release data. In order to process this, basic fission energy components and some composite components are defined.
- ENDF now offers three different options for fission energy release:
    i.   thermal point evaluation
    ii.   polynomial evaluation
    iii. arbitrary tabulated function. Added just a few months before the release of ENDF/B-VIII.0.
    Each of these has a slightly different way of storing the data in the ENDF file.
- Plots of the different evaluations were presented.
- KERMA calculations in the HEATR module were modified for the new data format
- NJOY allows you to specify whether you want to deposit the photon energy locally, or have it put somewhere else.
- In the future, we will separate as much as possible the contributions from all the particles.
- Fission must be handled differently because it is a special case for KERMA.
- Fixed a small inconsistency in the Sher-Beck (thermal point) calculation so you will no longer see a difference in the KERMA values for those situations.
- Several plots were presented showing the differences in the options and how they change the calculated KERMA.
- Changes have been made in NJOY2016 to take advantage of the new formats in ENDF/B-VIII.0.

Questions/Comments
- **Van der Marck**: Since I use NJOY/MCNP, I'm very interested in how HEATR is used on non-fuel pieces. Did you check the calculation for non-fissile material?
    o Not yet, but I intend to do this next year.
- **Van der Marck**: I've noticed that there are several evaluations that have negative heating values.
    o NJOY silently ignores the negative heating values. In a future release, NJOY will explicitly notify you that there is a possible problem and advise you to check the evaluation.
- **Kahler**: Unphysical heating values has been a problem for a long time. Bob MacFarlane has documented many of these issues on his website (legacy T2 website) going back many ENDF releases. The NJOY manual (see chapter on the HEATR module) also offers suggestions about what to check in the NJOY output.
- **Sublet**: Would it be useful to perform the same reporting of issues for ENDF/B-VIII.0 that has been done by MacFarlane?
    o It's a good thing to do, but is unlikely that anyone is really going to pay attention.
    o The ADVANCE server has done a lot of checking, but few evaluators are actually paying attention.

2.15. Benchmarking update on TENDL–2017, ENDF/B-VIII, JEFF–3.3, *S. Van der Marck*

- Automated the processing using:
    - NJOY2012.50 for ENDF/B-VIII.0
    - NJOY2016 (2 October 2017) for JEFF–3.3 and
    - NJOY2012.115 for TENDL2017 (by J.C. Sublet) (This is the same as NJOY2016.28.)
- Benchmark processing is intentionally dull and boring, you only change one minor thing and keep going
    - TENDL2017 builds upon many evaluations from ENDF/B-VII.0. TENDL has a goal of being "complete" so even though many evaluations come from ENDF/B-VIII.0, there are *many* more that are strictly from TENDL2017.
- Some plots were presented showing the critical benchmark differences between the three different libraries. Big differences are seen in:
    - LCT005 for JEFF–3.3. There is some gadolinium in these benchmarks which points to that evaluation that needs to be investigated.
    - The fast cross sections for nickel (in TENDL2017) may possibly cause some outliers
    - The tungsten evaluation in JEFF–3.3 may need to be investigated.
- The difference between the calculated and experimental value can be calculated, binned up, and compared to a normal distribution. In some cases, we seem to have significant biases. There are cases that all come from the same benchmark and are likely correlated. These calculations don't tell you what is wrong, but can point you to some evaluations that ought to be investigated.
- This analysis shows that for criticality calculations, TENDL2017 performance is getting closer to the other libraries, admitting, of course, that major evaluations come directly from ENDF/B-VIII.0.
- In addition to the critical benchmarks, shielding calculations were also performed and compared between the three libraries. All three libraries performed equally well except for two elements:
    - Iron (from TENDL2017) doesn't perform very well in LLNL pulsed sphere calculations. Haeck suggested the inelastic scattering and angular distributions are the cause for such differences.
    - Magnesium (from ENDF/B-VIII.0 and JEFF–3.3) doesn't perform well in LLNL pulsed sphere calculations. Inelastic scattering could also be the problem here that may date back to older versions of ENDF/B and JEFF.
- Beta-effective and Ross-alpha calculations show that the three libraries perform similarly.

Questions/Comments
- **Tada**: OECD/NEA WPRS is launching an effort to improve the quality of the description of the experimental data in SINBAD.

3. Action Items

- **Haeck** will fix GASPR to address issues identified by Sinitsa
- **Trkov** will continue comparisons with probability tables using ACE files that have already been collected from the participants.
- **Wiarda** will provide PENDF files (U-235 and U-238) with probability tables from AMPX that **Trkov** will convert to ACE files.
- Organize a follow-up meeting in approximately 12 months:
  - Stage 2 (self-shielding and probability tables) will be complete. Run suite of 32 ICSBEP benchmarks.
    - Analysis will be done with ACE files from different processing codes, but transported with MCNP.
    - **Trkov** will distribute ACE files and MCNP input decks
    - Codes that can use ACE files:
      - MCNP
      - MORET
      - OpenMC
      - Serpent
    - Codes that don't/can't use ACE files:
      - KENO
      - TRIPOLI
      - Mercury
    - Run Monte Carlo until k_{eff} is converged to < 10 pcm uncertainty
  - Preliminary Stage 3 (photon production in ACE files). Need to have photon production implemented in their ACE production code, at least a preliminary version.
    - **Trkov** will specify numerical benchmark that can be done as a fixed-source calculation
    - U-235 and U-238 from ENDF/B-VIII.0b4, everything else from ENDF/B-VII.1.
    - Reports about benchmarks from codes that run ACE files:
      - MCNP
      - Serpent
      - OpenMC
      - PHITS
    - **Trkov** will distribute ACE files that each code will use in the suite of 32 benchmarks.
    - For those codes that don't use ACE files:
      - TRIPOLI
      - MONACO
      - Mercury
      - Generate your own data and run
    - **Everyone** will present their benchmark results
  - Develop roadmap for comparison of thermal scattering processing and transport

- **Conlin** will have the document describing the continuous representation for thermal scattering ACE specification published
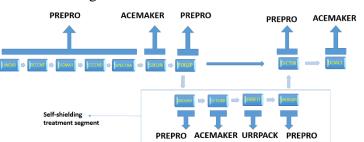
Appendix—Presentation Summaries

ACEMAKER: Treatment of self-shielding and new functionalities.

D. Lopéz Aldama, Agency of Nuclear Energy and Advanced Technologies, Havana, Cuba

The purpose of the ACEMAKER code package is to generate continuous energy ACE formatted files for Monte Carlo calculations from evaluated nuclear data files in ENDF/B format preprocessed by the PREPRO/URR-PACK package.

Figure 1 show calculation flow using PREPRO/URR-PACK/ACEMAKER package

Fig. 1: Calculation flow

The self-shielding treatment is based on the multiband approach presented in the following references:

- INDC(NDS)-0711, Rev. 1, "URR-PACK: Calculating Self-Shielding in the Unresolved Resonance Energy Range" by Dermott E. Cullen and Andrej Trkov, July 2016.
- Nuclear Cross Section Processing (D. E. Cullen), pp. 13-131, Vol. 1, in "Handbook of Nuclear Reactor Calculation", Yigal Ronen (Editor), CRC Press, inc., Boca Raton, Florida (1986).
- Nuclear Data Preparation (D. E. Cullen), pp. 279-425, Vol. 1, in "The Handbook of Nuclear Engineering", Springer Publishing, NY, NY (2010).

Nuclear theory predicts that the self-shielding will decrease with increasing energy as 1/E, so that the unresolved resonance region can be interpreted as a transition between the resonance fluctuations in the resolved resonance region, and the "smooth" tabulated cross sections at higher energies. Self-shielding factors (F-factors) are extrapolated from resolved to unresolved resonance range. From 2-band parameters, probability tables are prepared and added to the ACE-formatted file.

Photon production capabilities have been incorporated in ACEMAKER. Feature is under verification. The calculation is performed in the following way:

1. MF12/Option 2 (LO=2): Transition probabilities are converted to Option 1 (LO=1) production multiplicities
2. Photon data (cross sections, multiplicities, angular and energy distributions) are linearized in MF12, MF13, MF14, MF15 and MF6
3. Gamma production cross section is set equal to MF13+MF12*MF3+MF6*MF3

4. Prepare GPD, MTRP, SIGP, ANDP, LANDP, DLWP, LDLWP, and YP blocks in the ACE-formatted file.

In the future, it is planned to add thermal scattering law and dosimetry data processing to ACEMAKER as well as charge particle production.

Improvement of probability table generation using ladder method

K. Tada, Japan Atomic Energy Agency,

K. Tada presented the probability table calculation module of the FRENDY code. The FRENDY code uses the ladder method to calculate the probability table. The calculation methods of the complex error function and the Chi-Squared random number are modified to generate the more accurate pseudo resonance structure.

The complex error function is used to calculate Doppler broadened cross section using the ψ-χ method. Many calculation methods are developed to calculate the complex error function. The FRENDY code adopts three calculation methods, i.e., Algorithm 680, 4-pole Padé approximation, and the NJOY99 method. JENDL-3.3 has several nuclides which adopt the Single-Level Breit Wigner formalism in the resolved resonance region. These nuclides are used to investigate the prediction accuracy of the Doppler broadened cross sections using these calculation methods. The Doppler broadened cross sections using these methods are compared to those using with the kernel broadening method which is used in the BROADR (from NJOY) and the SIGMA1 (from PREPRO) modules. The calculation results indicate that the root mean square (RMS) values of the difference of all methods are similar. Since the approximation in the ψ-χ method is more significant than the approximation in the complex error function calculation, the difference between the two methods does not affect the difference of the Doppler broadened cross sections. Since the calculation time of the 4-pole Padé approximation is faster than that of the other method, the FRENDY code adopts the 4-pole Padé approximation to calculate the complex error function.

The Chi-Squared random numbers are used to determine the resonance width. Since the pseudo resonance structure significantly depends on the generated resonance widths, evaluation of the Chi-Squared random number is important. The NJOY and the U3R codes use the discrete random numbers to generate the Chi-Squared random numbers. The FRENDY code adopts the continuous random numbers to generate the rigorous random numbers. The mean, variance, skewness and kurtosis values of the both methods are compared. The skewness and kurtosis values of the discrete method have large difference. This result indicates that the discrete method cannot reproduce the shape of the Chi-Squared distribution.

^{235}U and ^{238}U from JENDL-4.0 is used to compare the probability tables generated by the FRENDY method and the NJOY99 method. The RMS values of difference are used for comparison. The number of bins is 20 and all cross-section boundary of probability bin are fixed in all cases. The comparison result indicates that the RMS value does not have a large impact on the results. The difference of the Chi-Squared random number generator does

not have a large impact on the probability table generation. The generation time of the FRENDY method is 20% faster than that of the NJOY99 method. Adoption of the 4-pole Padé approximation is effective to reduce the computation time. The k-effective values of the benchmark experiments in the ICSBEP handbook are compared to investigate the impact on the neutronics calculations. A continuous-energy Monte Carlo calculation code MCNP5 is used for this calculation and the sample input files of MCNP5 in the ICSBEP handbook are used. The benchmark experiments which have large sensitivity to the unresolved resonance region are selected. The k_{eff} values using the probability tables generated by the FRENDY method are similar to those by the NJOY99 method. The improvement of the Chi-Squared random number generation method also has no significant impact on the neutronics calculations.

The ladder number that is the generation number of the pseudo resonance structure has large impact on the computation time of the cross-section library. Therefore, the reduction of the ladder method is so important to reduce the computation time of the cross-section library. The probability tables in each ladder number are compared to investigate the appropriate ladder number. The ladder numbers for comparison are 10, 50, 100, 200, and 500. The ladder number for the reference case is 2000. The RMS values of the difference of the probability table are compared. The RMS values are small enough when the ladder number is 100.

Current Status on the Galilee-I code

C. Jouanne, CEA, Saclay, France

In the first part, many improvements made into the GALILEE-1 code are presented in relation to Andrej Trkov's comments for the ace files provided by GALILEE-1 in April. These modifications concern:
- the extension of the energy domain above 20 MeV in agreement with the evaluation file
- Doppler broadening for minor reactions, especially at low energy,
- linearization for narrow resonances (missing resonances using GALILEE-1)

Revised results presented show good agreement between PREPRO15, NJOY16 and the last version of GALILEE-1. New U235 and U238 ace files using GALILEE-1 for reconstruction in RRR and continuum energy ranges at 294K are available. The Probability tables are provided using PURR module and the ace file is assembled by the ACER module of NJOY16.

The second part of this presentation is dedicated to comparisons of calculations using TRIPOLI-4 and MCNP for criticality benchmarks with plutonium using the ENDF/B-VIII.0 library.

Significant differences are highlighted between these calculations with probability tables for TRIPOLI4 and MCNP (results from the publication of S. van der Marck). Using the ENDF/B-VII.1 library, MCNP (using PT from NJOY) and TRIPOLI-4 (using PT from CALENDF) are in very good agreement. The Pu239 URR cross-sections analysis shows

that the total section is not equal to the sum of the partial cross sections while the LSSF=1 flag is used. This induces an unexpected behavior within CALENDF that transfers this difference to the elastic scattering. By correcting the total cross section's evaluation (sum of partial cross sections), we observe a very good agreement for these criticality benchmarks between MCNP (with NJOY16 PT) and TRIPOLI-4 (with CALENDF PT). The verification of evaluation files is a very important step for the production of a nuclear data library.

The last part presents first results of PT calculations using GALILEE-1. The case studied is the Ba-140 from JEFF-3.2 library. The energy range is from 23 keV to 100 keV with constant parameters and LSSF=0. The temperature reconstruction is 0 K (no Doppler broadening). 20 000 sets of resonances are used to reconstruct PT at each energy given by NJOY16. 20 PT steps are calculated and inserted in a modified PENDF/PURR file. The CDF of total cross sections at one incident energy from PURR/NJOY2016 and GALILEE-1 are compared. They are quite different.

The ACER/NJOY2016 module is used to provide an ACE file. A very simple case is used to compare these new PTs. It is a sphere made of a single material. The neutron source is placed just above the unresolved domain (energy source at 105 keV). The response considered is the neutron flux in the sphere using a fine mesh. Several calculations are presented with very good agreement between them:
- MCNP calculation using NJOY2016 probability tables.
- MCNP calculation using GALILEE-1 probability tables.
- TRIPOLI-4 calculation using CALENDF probability tables.
- TRIPOLI-4 calculation using a translation of GALILEE-1 pointwise probability tables.

All these calculations are in rather good agreement, less than 3% when compared to MCNP calculations.

This is the first step in producing probability tables with GALILEE-1. The next steps will be taken in the coming year. We hope to be able to produce probability tables for MCNP in the unresolved range in 2019.

Processing GNDS for Monte Carlo and Multi-group Transport Codes

B. Beck, Lawrence Livermore National Laboratory, Livermore, California

LLNL has been updating its processing and transport codes to handle GNDS formatted data. The LLNL processing code FUDGE (For Updating Data and Generating Evaluation) can convert ENDF-6 and LLNL legacy ENDL formatted data into GNDS data. For GNDS data, FUDGE can reconstruct cross sections from resonance parameter and can heat cross sections. It can also generate multi-group files for all projectiles, targets and products for which data are specified. That is, FUDGE and, for that matter, GNDS are particle agnostic. FUDGE can transform GNDS evaluated data into a form better suited for Monte Carlo transport (e.g., place all cross sections onto a union grid, convert Legendre data into pointwise data, create cdf's from pdf's). FUDGE currently does not generate unresolved-resonance-region probability tables but this is being developed and will be available in next

release of FUDGE. In addition, GNDS currently does not have a way to store unresolved-resonance-region probability tables, this will need to be defined to support the next release of FUDGE.

LLNL has developed the C++ API GIDI (General Interaction Data Interface) that reads in GNDS files for use in transport codes. In addition to reading in GNDS data, GIDI provides routines to access multi-group data. Routines to collapse and transport correct multi-group data are also provided. LLNL has also developed the C++ API MCGIDI for use by Monte Carlo transport codes. MCGIDI extracts data needed for Monte Carlo transporting from a GIDI instance, puts the data into a compact form and provides routines to samples from the data. These include routines to sample a reaction and to sample the outgoing particles for a reaction. GIDI and MCGIDI will be released soon under a BSD license.

A FUDGE module toACE.py is being developed to generate ACE formatted files from GNDS files. Currently, toACE.py can produce neutron continuous-energy ACE files with outgoing neutron data (it does not produce the outgoing gamma data). However, toACE.py does currently generate unresolved resonance region probability table.

LLNL has a verification and validation (V&V) test suite designed originally to check evaluated data. Since the V&V test suite runs transport codes to calculate critical assembly k_eff values, reaction ratios and time of flight data (e.g., pulsed sphere experiments) against benchmark experiments, it is actually checking all phases required to produce the results: the evaluated data, the processing of the data and the transport code. LLNL has expanded its V&V test suite to allow for inter-code comparisons and comparisons of one data library against another. For example, the results produced using the data library ENDF/B-VII.1 can now be compared to the results produced using the data library ENDF/B-VIII.0. LLNL has also added testing designed to check that a processed file (e.g., ACE file) functions properly in a transport code. This was done to verify that the toACE.py module is generating properly formatted ACE files that produces acceptable results when used by MCNP.

Benchmark Calculations for U–235 and U–238 Multi-Band Data Based on ENDF/B-VII.1 and ENDF/B-VIII.0b4

D.H. Kim, Korea Atomic Energy Research Institute, Daejeon, Korea

D. Kim reported on benchmark calculations for U-235 and U-238 multi-band data based on ENDF/B-VII.1 and ENDF/B-VIII.0b4.

● Multi-band data processing
  • URR-PACK consists of two major modules, URRDO and URRFIT, to produce multi-band data for the unresolved resonance self-shielding treatment. URRDO can calculate multi-band probability tables from the NJOY-generated probability tables and URRFIT can calculate them from the original evaluated data.
  • The resulting 2-band probability tables from URRDO and URRFIT for U-235 and U-238 total cross sections were compared with the NJOY 20-band probability table. Both 2-band probability tables showed slightly different probability bin boundaries for U-235 and U-238. The probability tables from ENDF/B-VII.1 and

ENDF/B-VIII.0b4 showed similar tendencies but slightly large differences for 20-band and 2-band data originated from NJOY PTM.
- Criticality benchmark calculation results
  - The criticality benchmark calculations for 32 benchmarks have been carried out with three types of probability tables as well as the one turning-off PTABLE from 20-band probability table.
  - The C/E results with probability tables showed good agreements each other, but they showed large discrepancies for some IMF (e.g., BIG-TEN and ZPR-6/9) and MIF benchmarks when compared to the C/E results without probability tables. The discrepancies tend to be reduced for ENDF/B-VIII.0b4 compared to ENDF/B-VII.1.
  - The k-eff ratios by ENDF/B-VII.1 can reproduce the work reported in INDC(NDS)-0711 by D.E. Cullen well. Large self-shielding effects for some IMF and MIF benchmarks were observed due to U-235 and U-238 cross sections. For ENDF/B-VII.1, the results with the 2-band probability table from URRFIT showed differences larger than 0.1% for 3 BFS benchmarks compared to those with the 20-band probability table. For ENDF/B-VIII.0b4, all the 2-band results agreed well within 0.1%. Without unresolved resonance self-shielding, k-eff ratio differences between ENDF/B-VII.1 and ENDF/B-VIII.0b4 were up to ~0.1%.

Current status of the GAIA processing code

R. Ichou, IRSN, Paris, France

IRSN is developing a ND processing code, GAIA. Two versions of GAIA currently exist. GAIA 1, which is the current IRSN tool for nuclear data library generation, is designed to minimize the effort of generating nuclear data libraries (NJOY wrapper). It automates the entire NJOY 2016.35 processing path, but also performs a number of additional operations to verify the files and add any missing data. GAIA 2, a stand-alone C++ modular processing code project, is under development, and intends to be fully independent of NJOY (based on alternative methods). Different new methods have currently been implemented: mainly a Generalized R-matrix formalism (LRF=7) is used for RR reconstruction using R-matrix S-T decomposition and the use of Fast Fourier transforms for the Doppler effect, which allows for resonance reconstruction and Doppler broadening in a single step. IRSN is also currently working on new H2O thermal scattering data which could be fed into NJOYs LEAPR module, but can also be directly generated without NJOY (via a SAB module) to produce S (a, b). These new data are based on new TOF experiments at ILL and molecular dynamics simulations (Vaibhav Jaiswal PhD thesis). Another working area is the development of a new module for URR processing: the TOP module for 'Table Of Probability', which intends to replace PURR and improve the URR treatment (Clément Jeannesson PhD thesis). It is mainly based on the sampling of pairs of resonances around the reference energies (which is a method similar to the one in the PURM module of AMPX). It is also planned to work towards an analytical representation instead of probability tables. Finally, it is planned to improve the formalism for covariance generation in the next few years. A new GAIA scheme is proposed to be able to read both ENDF and GND formats and to include the new future modules.

IRSN performed the ENDF/B-VIII.0-beta4 U-235 and U-238 processing exercise, by using the PENDF produced by the resolved resonance reconstruction and Doppler broadening in a single step with GAIA, which was then fed into the NJOY ACER module. The cross-section results are in good agreement with PREPRO, but the data has some issues with the criticality benchmarks that were used in this study. This identified a bug in GAIA for threshold reactions that will be corrected.

Serpent and evaluated nuclear/atomic data

V. Valtavirta, VTT Technical Research Center of Finland, Finland

When the development of the Serpent Monte Carlo code was started in 2004 the main application of the code was to be simple reactor physics calculations, especially the generation of group constants for reduced order neutronics solvers. At that time the obvious reference code was MCNP and the obvious format for cross-section data was the ACE-format to allow comparisons between the two codes using exactly the same libraries. Since that time the applications of Serpent have diversified significantly requiring new data in addition to the one being readily available in ACE-files. On the other hand, some of the newer features of the ACE-format cannot have been properly utilized in Serpent due to the lack of publicly available format specification.

Despite some of the newer applications, e.g. photon transport, advanced heat deposition treatments and uncertainty propagation requiring data obtained from sources other than the traditional ENDF->NJOY->ACE sequence, the neutron interaction physics are still very much based on processing the ENDF-format files to ACE using NJOY. Furthermore, we see the more publicly accessible development and documentation of both NJOY and the ACE-format itself as very promising for the future of Serpent and all other ACE-users globally.

Resonance QA

D. Brown, Brookhaven National Laboratory, Brookhaven, NY

Dr. Brown described two codes useful for working with resonances. The first tool provides a capability to assess the quality of a given neutron resonance evaluation, with the goal of integrating the reporting tool into the ADVANCE continuous integration system. The tool consists of a Python script (grokres.py) which computes several metrics useful for quality assessment, particularly those sensitive to the two most common problems we see in neutron resonance evaluations: a) missing resonances and b) mis-identified resonances. These metrics consist of some things that are well known to practitioners of random matrix theory, but virtually unknown to the nuclear data community:

- Cumulative level distributions: these can be used to measure the average level spacing, D, and to search for deviations from the expected distribution which should be proportional to 1/D. These deviations signal missing resonances
- Plot of average level spacing, D, from both the RRR, and URR, to assess the consistency of the two parts of the full evaluation
- The resonance spacing distribution which is sensitive to missing resonances

- The resonance-resonance spacing correlation, which is sensitive to missing resonances, especially very close resonances
- The Dyson-Mehta Δ_3 statistic, which is exquisitely sensitive to both missing resonances and mis-identified resonances
- Plot of the mean resonance width, from both the RRR, and URR, to assess the consistency of the two parts of the full evaluation
- Plot of the width distributions which is sensitive to missing resonances

Using these, Dr. Brown was able to estimate the fraction of missing resonances in Fe-54 as well as other nuclei.

Knowing the fraction of missing resonances, Dr. Brown then proposed to use a second tool under development at BNL (mcres.py) to generate stochastic resonances. These stochastic resonances are completely consistent with the expectations of random matrix theory (not surprising as they are generated using the tools of random matrix theory). Dr. Brown plans to use these simulated resonances in a variety of roles including simulated resonance regions for off-stability nuclei, as a tool to generate resonance ladders for URR probability table generation, and to "back-fill" evaluations with missing resonances such as Fe-54.

Current State of AMPX

D. Wiarda, Oak Ridge National Laboratory, Oak Ridge, Tennessee

AMPX [1] is the processing system used in ORNL to produce cross-section libraries for use in SCALE [2]. AMPX is available as part of the SCALE distribution as of SCALE 6.1. AMPX does not produce libraries in the ACE format but instead the libraries are in a format native to SCALE and AMPX. Currently all kinematic data are given in the LAB system. AMPX has been developed since the early 1970 but many of the modules have been rewritten in modern C++ with a well-defined API conforming to a SCALE standard. AMPX as well as SCALE follow a strict QA procedure for developing and testing the code. AMPX can produce coupled CE and MG libraries as well as various decay libraries for use in the depletion calculations. Covariance libraries can also be generated. CE, MG libraries in various group structures and covariance libraries have been generated from ENDF/B-VIII.0. These libraries are currently undergoing testing for release with the upcoming SCALE 6.3 beta release.

For ease of use AMPX includes a graphical user interface (GUI). Templates exists for all the library types produced. Templates are keyword based input files that take user information such as the group structure, the flux to be used for collapsing. These templates are then expanded into AMPX input files. The GUI can queue the input files on one or more nodes of a compute cluster or on a single machine, if a native queuing does not exist. The GUI also allows to examine all AMPX input files.

For use in MG shielding calculations AMPX generates Bondarenko factors for various temperatures and background cross sections. Initially factors are generated in a narrow resonance approximation. SCALE allows to run a point-wise shielding calculation in the resolved range, which is then collapsed back to MG format for use in the subsequent

transport calculation [3]. Since these calculations can be time consuming, we pre-calculate the shielded cross section for an infinite homogenous cell at different temperatures and background values and save the data back as updated Bondarenko factors. This is done for nuclides with a Z > 39. Shielding factors are also calculated for the diagonal of the elastic scattering matrix.

AMPX includes an ENDF library that reads (and writes as needed) ENDF data. In this library, ENDF data are read into in-memory structures and all subsequent modules only access these in-memory structures. Currently, the library only reads ENDF-6 data. However, work is progressing to extend this to GNDS data. GNDS reading is currently supported for 1-D data for incident neutron (includes resonance data) and covariance data. This functionality will be released in beta form with the upcoming SCALE 6.3 beta release. We are also planning to use the same ENDF library in SAMMY [4], the ORNL Nuclear Cross Section evaluation tool. This will allow AMPX to use all the updated resonance calculations tools in SAMMY and will allow SAMMY to use the new GNDS features in the resolved resonance range.

[1] D. Wiarda, M. L. Williams, C. Celik, M. E. Dunn, *AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications*, International Conference on Nuclear Criticality Safety (ICNC 2015)
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[3] M. L. Williams, *Resonance Self-Shielding Methodologies in SCALE 6*, Nucl. Technol. 174, 149 (2011).
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Updating NJOY's HEATR module for ENDF/B-VIII.0

W. Haeck, Los Alamos National Laboratory, Los Alamos, New Mexico

This presentation mainly dealt with the changes made to the HEATR module in NJOY2016 following the introduction of the arbitrary tabulated function format for fission energy release components in ENDF/B-VIII.0. This work is an example of how things should proceed within NJOY21: starting with a detailed review of the existing NJOY code, being corrected where it is deemed required and supplemented with additional methods. Detailed documentation on the various methods and V&V testing should also be made available.

Each release of the ENDF/B library often results in the introduction of new data formats in the ENDF-6 format. With ENDF/B-VIII.0, which was released in February 2018, new formats were added for allowing tabulated fission energy release components in the MF1/MT458 section, to allow for sub-actinide fission and non-neutron induced fission in the MF8/MT18 and MF10/MT18 sections, and to add fission neutron and gamma emission probabilities in the MF6/MT18 section. Processing codes must be adapted to ensure that they are capable of using these new data, or at the very least understand the new formats.

NJOY2016, a nuclear data processing code developed at Los Alamos National Laboratory, is no exception to this.

Evaluated data for the fission energy release components have been available in the ENDF format in section MF1/MT458 since its introduction in the ENDF-5 format in 1983. Today, the MF1/MT458 section allows an evaluator to describe these components and their energy dependence in three different ways:
- the thermal point evaluation using Sher and Beck energy dependence systematics (the original ENDF-5 format);
- the polynomial evaluation using polynomial energy dependence systematics (introduced in the ENDF-6 format in 2010);
- the tabular evaluation using tabulated energy dependence (introduced in the ENDF-6 format in 2017).

Changes were made to MODER to be able to read the new section when changing between ASCII and binary mode. The introduction of the tabulated fission energy release components also requires changes in HEATR so that these new data can be used. The implementation in the HEATR module was also changed so that all format types are used consistently. Previously, evaluations using thermal point used a slightly different equation so that older versions of NJOY will now give slightly different heating values (differences of the order of 0.1% can be observed for most energies, at energies above 10 MeV this can be up to 1%). The polynomial type still yields the same values (the implementation has changed somewhat but the actual formula that is used was not).

Benchmarking update on TENDL–2017, ENDF/B-VIII, JEFF–3.3

S. van der Marck, Netherlands

In the last year, new versions have been released of the nuclear data libraries ENDF/B, JEFF, and TENDL. This provides a nice opportunity to assess the current capabilities of neutron transport codes to simulate nuclear processes when using these modern libraries.

Between a nuclear data library in ENDF or GNDS format and the actual use of these data in a transport code, there is the issue of 'processing', the subject of this Technical Meeting. Several versions of NJOY were used to process the various libraries, reflecting the timing of the release of each library. ENDF/B-VIII.0 was processed with NJOY2012.50, JEFF-3.3 with NJOY2016.20 and TENDL-2017 with NJOY2016.28. In the case of TENDL all files were also processed with NJOY2016.20, and the benchmark results showed negligible differences.

Many benchmarks were run for each of the nuclear data libraries:
- 2528 criticality safety benchmark cases from ICSBEP;
- 68 shielding benchmark cases from SINBAD;
- 32 test cases for delayed neutrons (β_{eff} and Rossi-α).

All results are scheduled for publication or have already been published: D. Brown et al, Nuclear Data Sheets 148 (2018) 1–142 and M.B. Chadwick et al, Nuclear Data Sheets 148 (2018) 189–213 for ENDF/B-VIII.0, O. Cabellos, to be published in European Physics

Journal 2018, for JEFF-3.3, and A.J. Koning, to be published in Nuclear Data Sheets 2018, for TENDL-2017.

Overall the three libraries show similar performance in the overwhelming majority of the benchmarks. In some cases, differences can be noticed.

- In LEU-COMP-THERM-005 the results based on JEFF-3.3 are higher than the results based on ENDF/B-VIII.0 or TENDL-2017. Some effort is required to establish the cause of these differences, but it may be related to the Gd evaluations.
- The results based on TENDL-2017 for the LLNL Pulsed Sphere shielding benchmarks with Fe are different from those based on ENDF/B-VIII.0 or JEFF-3.3. The performance of the latter two libraries is better for these cases.
- The results based on TENDL-2017 for the LLNL Pulsed Sphere shielding benchmarks with Mg are different from those based on ENDF/B-VIII.0 or JEFF-3.3. The performance of TENDL-2017 is better for these cases.

Technical Meeting on Nuclear Data Processing

IAEA Headquarters, Vienna, Austria
3 – 6 September 2018
Meeting Room VIC C5 (7th floor)

Preliminary AGENDA

Monday, 3 September

08:30 – 09:00   **Registration** (IAEA Registration desk, Gate 1)

09:00 - 09:30   **Opening Session**

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

09:30 - 12:30   **Presentations by participants** (~ 30 min' each)

1. *Verification of GRUCON Modules and Calculation Procedures for ACE File Generating*, V. Sinitsa

2. *ACEMAKER: Treatment of self-shielding and new functionalities*, D. Lopez Aldama

3. *Improvement of probability table generation using ladder method,* K. Tada

4. *Current Status on the Galilee-1 code,* C. Jouanne

12:30 – 14:00   *Lunch*

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

5. *Progress on ACE file prcessing of RULER*, P. Liu

6. *Processing GNDS for Monte Carlo and Multi-group Transport Codes*, B. Beck

7. *NJOY Status in 2018*, J. Conlin

8. *Benchmark Calculations for U-235 and U-238 Multi-Band Data Based on ENDF/B-VII.1 and ENDF/B-VIII.0b4*, D.-H. Kim

Coffee breaks as needed

Tuesday, 4 September

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

    9.   *Current status of the GAIA processing code,* R. Ichou
    10.   *Serpent and evaluated nuclear/atomic data*, V. Valtavirta
    11.   *Resonance QA*, D. Brown
    12.   *Results of ACE Library Code Verification Project - Stage 1,* A. Trkov
    13.   *Benchmarking update on TENDL-2017, ENDF/B-VIII.0, JEFF-3.3,*
           S. van der Marck

2:30 – 14:00   ***Lunch***

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

    14.   *Current Status of Ampx*, D. Wiarda
    15.   *Updating NJOY's HEATR module for ENDF/B-VIII.0,* W. Haeck

Coffe breaks as needed

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

Wednesday, 5 September

09:00 - 12:30   **Round table discussion**
                 Discussion on the presentations

12:30 – 14:00   ***Lunch***

14:00 – 17:30   **Round table discussion** (cont'd)
                 Drafting of the Summary Report and Action List

Coffee breaks as needed

Thursday, 6 September

09:00 - 16:00   **Drafting of the summary report** (cont'd)
                 Finalisation of the Summary Report and Action List
16:00   **Closing of the meeting**

Coffee break(s) and lunch in between

Technical Meeting on
Nuclear Data Processing

3 to 6 September 2018
IAEA, Vienna

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