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SUBJECT: Report on Foreign Travel to IAEA Meeting on Nuclear Data Processing
DATE: 1/30/2023
TO: Dr. Angela Chambers, Nuclear Criticality Safety Program Manager, National Nuclear Security Administration / NA-511
FROM: Wim Haeck, LANL

MEETING TITLE: Technical Meeting on Nuclear Data Processing

MEETING LOCATION: Vienna, Austria

MEETING DATES: 29 November to 2 December 2022

ATTENDEES ON BEHALF OF NCSP: Wim Haeck

MEETING PURPOSE: The purpose of the event is to review the results of the processed library inter-comparison exercise as a follow-up to previous meetings.

The meeting consisted of presentations on the status of all nuclear data processing codes available in the world. This includes AMPX from ORNL, GALILEE from CEA (France), GAIA from IRSN (France), Fudge from LLNL, Frendy from JAEA (Japan), Grucon (Russia), etc. In particular, the meeting focused on the results from the thermal scattering intercomparison (continued from last year) but a number of additional subjects were touched upon:

- Resonance reconstruction: discussion on a more detailed and focused intercomparison (i.e. very simple cases that can be solved analytically to very complicated cases). I personally pushed for this since I would be able to use these cases for testing our modernized resonance reconstruction tool.
- Blatt-Biedenharn to calculate angular distributions from resonance parameters
- Anisotropic fission: apart from a few exceptions, current evaluations for fissionable nuclides have always assumed fission neutrons to be isotropic. At higher incident neutron energies and the higher outgoing energy range, this is not entirely correct. Evaluations like Th have angular distribution data in it for fission neutrons, and the data is added to the ACE file.
- Doppler broadening: discussion on algorithms, where to end Doppler broadening, Doppler broadening of angular distributions

MEETING BENEFITS TO THE NCSP: The meeting directly relates to ongoing work funded by the NCSP for Nuclear Data processing and preparation of the data for use in analytical methods.

PURPOSE OF TRAVEL
Attend IAEA Technical Meeting on Nuclear Data Processing at IAEA, Vienna

Persons Contacted at IAEA
N/A

Presentations, Chair Responsibilities, Etc.:
Wim attended upon invitation from IAEA and give a presentation, He was also chosen as rapporteur along with Andrej to develop the notes:

Participants introduced themselves. Arjan gave a background discussion on why the meeting exists including a history of the status of various processing codes. Inter-comparisons are an ongoing effort in order to keep the codes in good shape (correct, with modern implementations and physics).
Reviewed agenda, elected chair and rapporteurs. Andrej was elected chair, rapporteurs were chosen to be Andrew and Wim. Two presentations were added to the agenda for the second day of the meeting.
Roberto proceeded to lecture on the topic of where problems in the evaluation should be fixed – is the responsibility on the evaluator producing the file or on the processing codes to fix the problems? When the processing code fixes it, there is ambiguity, so that the inter-comparison of the codes is necessary; regardless of choice we should make sure that the processing from any code should produce approximately the same cross sections. The ambiguity implies something wrong with the evaluation or the format definition, and in either case it should be fixed so that the results of nuclear data processing are unique.
Inter-comparison of the nuclear data itself is important because we need to understand where the differences in the transport code results are coming from. Neutron induced data has been extensively tested and used but now as application needs arise that use incident particles other than neutrons we need to continue the inter-comparisons for the other data types as well.

Chair Andrej took the floor, we dealt with audio-visual questions, and opened the meeting, reiterating the importance of these cross comparison exercises. He ceded the floor to our first presenter, Do Heon Kim to speak about Nuclear Data Processing and Validation at KNDC: H in ZrH and IAEA/PD-2019.

Mr. Kim spoke about his V&V sensitivity study of “H in ZrH”. Comparisons of incoherent inelastic scattering cross sections were performed using IFENG=2, 32 angular bins, emax=10 eV, and a tolerance of 0.3%, maximum k-eff MC uncertainty was 10-20 pcm. A suite of 10 benchmark problems was tested taken from the ICSBEP handbook, all of which require the H-ZrH thermal scattering law data. These inputs also required TSL data for Zr-ZrH, H-H2O, b-beo, others and Fe-56 and Al-27 taken from ENDF-7.1. IFENG=1 vs 2 can lead up to 300 pcm change for one benchmark, less than 100 pcm the rest of the inputs. NBIN=16, 32, 48, 64 are less than 40 pcm for all benchmark problems tested in the suite. Differences seem to increase for NBIN > 64 so we should test for larger NBIN. Emax did not have a strong impact on benchmark cases considered. Need to check for TOL < 0.1%.
Mr. Kim next spoke about the photonuclear data productions under IAEA CRP. KAERI contributed 124 of 164 nuclides in the library for CRP 1999. Second CRP 2019 has 219 nuclides with 30 nuclides contributed by KAERI. Both sets were processed with NJOY-2016 and tested with MCNP-6.2. Two old measurement photon-neutron yield benchmarks were used to perform testing of the data. One has C, Al, Cu, Ta, Pb, U as targets with various thicknesses in radiation lengths (RLs) at different electron energies. The second has a semi-infinite slab geometry and targets of Al, Fe, Cu, …

Swanson theoretical benchmark generally agree well except for Al and W at 15 MeV. For Cu and Ta targets, all agree well. Pb targets show similar results but for W targets yield was low. ENDF7U and ENDF-8 almost identical.
Barber & George: [I missed the first slide but I think there was nothing remarkable, things compared well.] For Cu results agree well at 16.1 and 21.2 MeV, at higher energies the differences are larger but within benchmark uncertainties. At higher energies the difference decreases. For lead targets up to 6 RLs shows good agreement across entire energy range. END7U and ENDF8 are identical and better than LA150U and IAEA/PD-2019.
Discussion afterwards discussed the importance of Mr. Kim's testing numerical testing as well as comparison to measured data, potentially highlighting the deficiencies in the photo-nuclear library that are simply due to measurement deficiencies. Photo-nuclear measurements at RPI with tantalum are not able to be reproduced well by simulation results. Andrej requested that the MCNP inputs and results should be shared with the group to potentially be used by the community as a photo-nuclear benchmark. Roberto pointed out that the IAEA has Bremmstralung spectrum database (useful for LINAC modeling), noting the inverse behavior of the spectra with the cross section at the lower energy range. It was also noted to be careful with the version of MCNP used as there is a certain scattering law description that is not able to be used in some versions.

Mr. Kahler presented next on a comparison of keff results for some TSLs with an enhanced "egrid." Skip clarified the use of EMAX in THERMR and how it is behaved. Default cosine bins and spectral convergence was 32 and 0.3% respectively. Currently there is not an option in NJOY to specify the outgoing energy grid. MCNP uses free-gas approximation above the thermal. Skip clarified what NJOY does to explain how it interprets the different user options in conjunction with the data available in the TSL data. Legacy 118 points output, egrid option used to make 469 point grid (roughly 3 points added between the legacy grid points). Tested for H-ZrH, H-H2O, H-CH2, graphite TSL data with benchmarks containing those TSL data.
For H-ZrH: Positive bias for increasing EALF, no change for most low EALF, TRIGA reactor is an exception with a negative bias for the denser grid (calculated as 4x grid result – legacy grid result). EMAX=10 eV will make NJOY use short collision time (SCT) up to 10 eV rather than free-gas treatment between 1.85 eV and 10 eV (what MCNP would have filled in). The effect of dense output grid and change in free-gas for SCT should be provided to see the combined effect.
For H-H2O energy grid density has no impact on k-eff. Behavior is similar for H-CH2 and graphite. No difference for H-H2O EMAX because it did not change the results of the processing.
Mr. Kahler reiterated the importance of understanding the choices made when processing and the behavior that implies when it is used in the transport code (free-gas vs SCT).
Discussion: The group then discussed the importance (especially for oscillatory cross sections in the eV range, like hydrides) to have an adaptive grid or a denser grid to capture the TSL physics to a sufficient accuracy. Wim stated NJOY is going to allow a user-provided grid to allow the user to optimize the refinement to their own needs, and if time permits an adaptive grid will be implemented. Skip pointed out that it is ambiguous (once outside of the energy provided in TSL file) if it is intended that free-gas or SCT should be used; CSEWG handbook says to use SCT rather than free-gas outside of that range. Andrej mentioned that some of this issue of ambiguity is avoided if the evaluation goes to a higher energy to begin with. Roberto wanted to stress that the dual recommendations is to go higher in energy for the proliferation of TSL data but also ensure that when the treatment switches that it is smooth. Doro pointed out that it is also important to communicate how the TSL data (elemental) is supposed to be bound to its isotopic components. Even if it can be processed, need to communicate this to users to be able to use the data correctly! Need a better classification system for what to use and when as the use (or non-use of) TSL data can have a huge impact on computational results. Discussed a bug with MCNP

using fissionable TSL materials. Andrej asked that the report detailing the bug be distributed to the community (LA-UR-21-21189). Dan discussed that normal users do not have the skills to modify the TSL data to actually create the nuclear data needed for their application problem correctly. Dan talked about a logical disconnect between the evaluation and NJOY EMAX, what is intended versus what people (novice and advanced) will do with their processing. Roberto emphasized the need to communicate to the evaluator community to make sure that their evaluation provides a smooth transition regardless of the choice of processing.

Mr. Tada (JAEA) took the floor to speak on the recent developments in the FRENDY processing code. FRENDY version 2 was released in January 2022 and is open-source. FRENDY now creates multigroup cross sections and provides uncertainty quantification in URR with uncertainty in probability tables. Version 2.01 was released in November 2022 with developments including DBRC, MG data for secondary gamma spectrum, and a linearization function for tab1 data. For resonance up-scattering correction (RUC) mixed nuclide resonance interference effects can be modeled for example U-235, U-238 with RUC and O-16 without RUC. Samples for use are provided in the manual. FRENDY MG secondary gamma spectrum shows good agreement with NJOY results and is available for a large variety of ENDF-formatted data libraries. For 2D data FRENDY uses method of corresponding energy (MCE) rather than unit-based interpolation but gives equivalent results as unit-based if the number of subdivisions is 1 (but the default for FRENDY is 2, further increasing this number did not significantly change the distribution compared to using 2 subdivisions). According to Mr. Tada, for TAB1 data with multiple interpretation schemes applies the first interpolation schemes to all sections, whereas FRENDY correctly uses the scheme specified for each section of the TAB1 data; ergo, the linearization function added to FRENDY is used to force all of the data in the evaluation to be linearized. The linearization function in FRENDY produces identical results to the NJOY RECONR results. The publication of the FRENDY manual is forthcoming, wants to add KERMA and damage calculations to FRENDY, and process covariance data.
Discussion: [seems unrelated to presentation at hand] Red asked about LRF=7 with SHIFT=1 (calculate shift rather than assume S(E)=B). Cu-63 file was provided for testing to make sure that the codes calculated correctly. Andrew gave very astute comment on why this is desirable (B=-l vs B=S(E)) where the resonances appear at energies that correspond to their resonance parameters (rather than being shifted off).
[seems unrelated to presentation at hand] Red also mentioned something about there being an ambiguity with the LRF=7? It was unclear what was ambiguous about the format and Red was unavailable for comment.
Oscar asked about the availability of the DBRC being implemented in the transport code versus the processing code. Mr. Tada explained that the modifications were done such that FRENDY could provide the data required to perform the DBRC calculations in the transport code (not in FRENDY). Dan clarified that the issue of DBRC is trickier for multi-group data as probability tables for that must be provided (versus elastic 0K data for CE MC codes).

Mr. D. Lopez Aldama presented on some development of IAEA tool that improve processing for the URR, TSL, dosimetry, and photonuclear data. ACEMAKER is open source and is available on the NDS/IAEA github page. ACEMAKER prepares ACE-formatted files for CE neutron, CE photo nuclear, dosimetry, and S(a,b). Previously, the IAEA tool was using averaged parameters from the resolved resonance range, extrapolated to the unresolved energy range (performance was poor for Ta-181). There are now new formulas implemented which are still approximate and provide averaged parameters but are reproducing the behavior much better when extrapolated to the unresolved resonance range.

Differences were then demonstrated for actinides and Ta-181 compared to unshielded values, M0 shielded values, and M1 shielded values. All three approach the same value as the energy increases into the smoothly varying high-energy region (above resonant). For TSL, an adaptive incident energy grid has been implemented. The results presented here for the benchmarks with H-ZrH agree with the findings by Mr. Kahler. For dosimetry, there is now the ability to prepare production cross sections for MF3, MF10, MF3/MF9, and MF3/MF6 in ACE format and X-Y tables. There is an input option to force the calculation of production cross sections from MF3/MF6. For photonuclear data, processing now correctly includes production cross sections from MF3(MT201-207), MF10, and MF6/MF3 combinations; also processes MF12 and MF14; correct treatment of MF6 (LAW2/LAW4) combination; treatment of recoil nuclear when it is a particle with ZA <= 2004; processing of delayed neutron spectra from photofission; includes relativistic conversion between CM and LAB for heating calculation. [Discussion about the NJOY treatment of the MF3(MT201-207) and the behavior compared to the results presented here, it seems to point to NJOY not doing the right thing in this particular case. Wim suggested that checking for these problems before processing would be good to ensure that this is in fact what the evaluator intended and that it is not a problem in the evaluation. Andrej suggested that this can be guarded against in the processing codes for derived data files (consistency check with MTs available on the file). Andrej mentioned that covariance data (particularly partials) have the same sort of problem. Redundant information in the file or not, what takes precedence?] Also for photonuclear data, production cross sections required extending MTD (which means to use them it needs an MCNP update) rather than using the extended MTD values, a set of temporary MTD have been set to fulfill users' requests, (MTD=219-451, 461-599, 850-874, …). IAEA/PD2019 photonuclear library was processed using ACEMAKER, and the processed files are available on the NDA/IAEA github page. The availability of the processed data has allowed the calculation of the production of medical radioisotopes. [Discussion: Andrej asked Wim to pass the request to the MCNP developers to fix the problem with MTD being limited to <999. Wim will follow up. Roberto mentioned some problems with intermixing transport and dosimetry libraries. It was suggested that an elegant solution to this problem may be to modify the header portion of the ACE file.] MCNP is not using anisotropic neutron emission from Ta-181, important above 3.5 MeV. [Discussion: Might be that MCNP is not understanding LAW61 or that it is assuming isotropy at that energy.] For IAEA/PD2019 evaluation purposes there are issues with:

- 2-He-3 using LAW=2 for deuterons
- 4-Be-9 considers reactions MT32, 35, 41 as break-up reactions
- for 6-C-12 total inelastic reaction MT=3 does not match sum of partials below 1.6 MeV
- 7-N-14 evaluation specifies MT=118 as break-up but this is an extension of ENDF-6 MT definition
- 50-Sn-118 non-monotonic energy grid for MT201
- there is an incorrect first incident energy for the yields for 67-Ho-165, 69-Tm-169, and 73-Ta-181
- the energy angle distributions for tungsten are unrealistic
- 13-Al-27 incorrectly sets LCT=1 for Kalbach-Mann formalism

The future work is to add charged particle processing, further improve URR treatment, improve damage and KERMA calculations, covariances, update documentation, V&V (next release planned in January 2023).

Discussion: There is a general problem with checking codes, the format, and processing codes getting out of sync. We will discuss more the talk later when we have more time.

Ms. R. Ichou presented the status of the GAIA-2 processing code at IRSN. GAIA-2.1 is under development at IRSN which allows two processing routes: 1) GAIA-1.3 is a wrapper around NJOY and adds any missing data and is the current processing tool for library generation at IRSN, or 2) a tool developed at IRSN. A

flowchart showed the working of the GAIA-1.3 system wrapping the various NJOY processing steps. The GAIA-1.3 system is used to process files for MORET, VESTA, and to produce all of the CE libraries for MCNP, MORET, VESTA, SERPENT for many evaluations (e.g. JEFF-3.3). Flowcharts were presented demonstrating the differences in the scheme between GAIA-1.3 and GAIA-2.0; in the end both output ACE files for isotopes and TSL data. GAIA-2 is in C++ with modules DOP (Doppler and resonance reconstruction), TOP (URR treatment), SAB (TSL treatment), COV (to be done by PhD thesis, improved formalism for covariance generation). The DOV module is able to process LRF=7, including producing the angular distributions. DOP solves the Doppler broadening equations using a fast fourier transform approach. TOP implements a standard probability table treatment in the URR, and average cross sections can be calculated from the probability tables according to the Hauser-Feschbach formalism to calculate a width fluctuation correction factor. SAB can only process H-H2o, H-CH2, and H-HF but is able to interpolate between the frequency spectra to generate TSL data at arbitrary temperatures. GAIA-2 future plans include developing the COV module (improved formalism generation and angular distribution uncertainties), V&V the processing, create activation libraries, implement GNDS reading, further enhance SAB capabilities, replace ACER and HEATER. With regards to the U-235, U-238, Cu-63 exercise: U-235, U-238 processed with no issue. GAIA-2 could not process Cu-63 file due to ISHIFT flag. Falling back to RECONR processed fine AFTER MF32 was removed from the file (otherwise it failed) Discussion: Andrej suggested that this is probably due to a problem with multiple MT34. Wim informed us that MODER converts the entire ENDF file to binary format so it is possible the error is due to the file being malformed or the conversion not implementing the translation correctly for some section of the file. Wim explained how the FFT is applied to the 0K data to get temperature broadened data. All agreed that regardless of how the Doppler broadening is carried out it should give the same results as the more traditional methods. Discussion about the details of the particular implementation was discussed, it would be good to know more about the details including the number of points and the time it takes to compute compared to the traditional approaches.

Andrej thanked the speakers and closed the meeting.

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