Brookhaven National Laboratory

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CSEWG Meeting Minutes

31 October - 4 November 2022

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U.S. DEPARTMENT OF ENERGY

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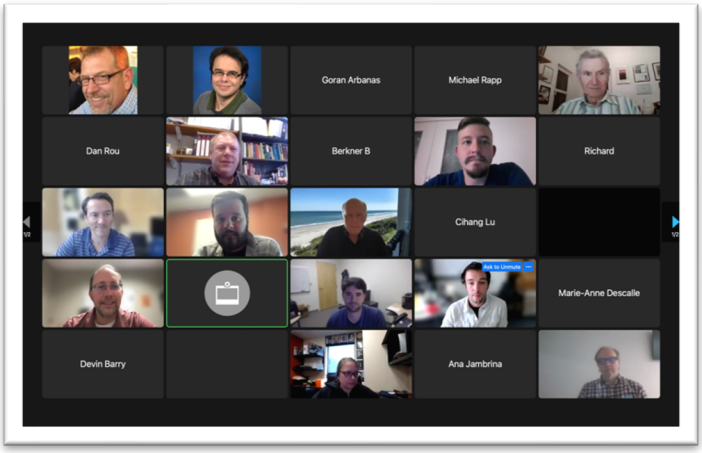
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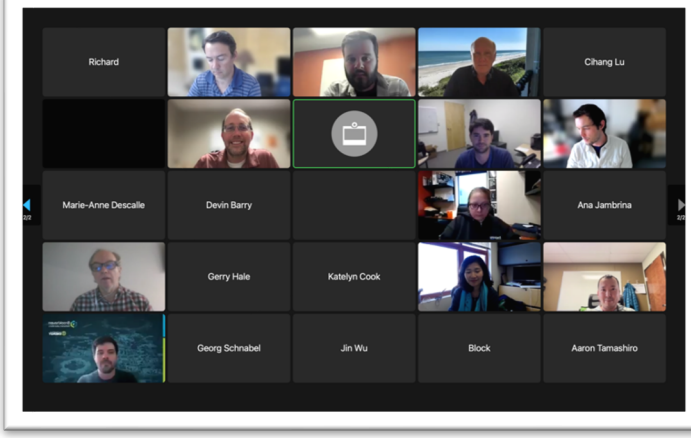
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Special Thanks

Meeting Organization

David Brown (BNL, NNDC Head, CSEWG Chair)
Gustavo Nobre (BNL, ENDF Library Manager)
Letty Krejci (BNL)
Ana Popovici (BNL)

Meeting Rapporteurs

Peter Brain (RPI)
Katelyn Cook (RPI)
Greg Siemers (RPI)
Suk Singh (RPI)

CSEWG Committee Chairs

Evaluation [Transport and Neutrons]: Mark Chadwick (LANL)
Evaluation [FPY and Decay]: Toshihiko Kawano (LANL)
Evaluation [TSL]: Ayman Hawari (NCSU)
Evaluation [Charged Particles]: Marco Pigni (ORNL)
Data Validation: Mike Zerkle (NNL)
Formats and Processing: Mike Dunn (Spectra Tech Inc.), Doro Wiarda (ORNL)
Measurements: Yaron Danon (RPI)
Covariances: Denise Neudecker (LANL)

CSEWG Executive Committee Meeting

Chair: Brown David (NNDC, Brookhaven National Laboratory)
Date: Tuesday, November 1, 2022

The CSEWG executive committee met to discuss several items: the executive committee Sharepoint site, the next CSEWG and mini-CSEWG meetings, representation at WPEC, the possibility of adding an at-large member to the CSEWG executive committee and a path forward for the ENDF/B-VIII.1 239Pu evaluation.

CSEWG meeting: *The next CSEWG/Nuclear Data Week meeting will be the week of November 13th, 2023*. This avoids both the Winter ANS meeting and the APS-DNP meeting. The meeting will be most likely hybrid, but with a much larger in-person attendance than this year's Nuclear Data Week. We will attempt to replicate the success with the RPI rapporteurs (who are amazing!). The details over whether we will need to charge a registration fee to cover coffee, etc. has yet to be worked out. There is also the question if we can have an unhosted dinner to function as a "release party" for ENDF/B-VIII.1. There was agreement that student participation should be free.

Mini-CSEWG meeting: It was decided that we will hold a mini-CSEWG meeting before the planned Beta2 release in June. Given the WPEC meeting timing, WONDER and Varenna meetings, and the ICSBEP meeting from April 3-7, the best time appears to be mid-to-late April or late May. The executive committee still must pick a time and a host institution.

WPEC & Subgroups meeting: There was a motion to expand our participation in the HPRL. Also, it was announced that C. Mattoon (LLNL) is now the chair of the GNDS Expert Group.

ACTION: D. Brown will reach out to A. Holcomb (OECD/NEA) to nominate Hye-Young Lee (LANL) and Mike Zerkle (NNL) to the HPRL Expert Group.

At-large member: There was a proposal to add Roberto Capote as an at-large member of the CSEWG executive committee to function as an information INDEN liaison. This was discussed at the meeting and agreed to at the subsequent CSEWG executive committee teleconference on December 1st.

Proposed 239Pu plan (for beta1), giving testing constraints: Given the short timeline between Nuclear Data Week and the planned ENDF/B-VIII.1 Beta1 release, the executive committee needed to decide on a path forward for the ^{239}Pu evaluation to be included in Beta1 for testing. As a reminder, ENDF/B-VIII.1 currently has three candidate evaluations, from the INDEN collaboration, from LANL and from LLNL. Arguably all three (LANL, LLNL and INDEN) variants are substantially better performing than the ENDF/B-VIII.0 evaluation. After much debate, the executive committee voted to create a hybrid evaluation from the three evaluation efforts. The decision was not unanimous (6 for, 2 against and 6 abstentions). The biggest argument against a hybrid evaluation was that it destroys the consistency between the different channels. On the other hand, such a hybrid capitalizes on the best elements of each evaluation effort. In any event, having results for the performance of this hybrid evaluation during the spring (and reported at the mini-CSEWG meeting) will allow time for refinements in Beta2. The components of the hybrid evaluation are:

- Inelastic and elastic from LANL (+LLNL). The LANL evaluation has potentially better pre-equilibrium modeling

- Capture cross section from INDEN because of the inclusion of Hopkins and Mosby data and a careful review of other datasets
- (n,2n) from INDEN, because of the use of the Lougheed 14 MeV points. It was noted that careful consideration of GEANIE partial gammas may give better threshold behavior
- RRR from prior ORNL work used in the pre-CSEWG meeting evaluations
- PFNS from LANL used in the pre-CSEWG meeting evaluations
- The Nuclear Data Standards (n,f) cross section

In addition, LLNL volunteered to assemble the evaluation in parallel with the IAEA to ensure that the final evaluation is reproduceable.

Validation Committee

Chair: Mike Zerkle (NNL)
Date: Monday, October 31, 2022

Welcome

Speaker: Brown David (NNDC, Brookhaven National Laboratory)

Overview: Welcome to everyone! ENDF/B-VIII.1 beta release is coming soon.

Introduction

Speaker: Michael Zerkle (Bettis Atomic Power Laboratory)

Overview: Validation session includes 9 presentations.

Validation of ENDF/B-VIII.1-/beta-based continuous-energy data tables

Speaker: Noah Kleedtke (LANL)

Overview: Work has been done at LANL to validate various updated evaluations from ENDF/B-VIII.1b0 including: Fe, Cu, Si, U, Pu. Continuous energy tables were processed with NJOY2016 and output to ACE files. For non-Pu legacy critical benchmarks, all calculations were within the experimental benchmark uncertainty, with some benchmarks having shown lower bias using ENDF/B-VIII.1b0. In HST systems, ENDF/B-VIII.0 shows reasonable results above the thermal leakage fraction. ENDF/B-VIII.0.1 is doing slightly worse than ENDF/B- VIII.0. b0.2 and it also includes a new ^{19}F evaluation, so more work is needed to examine its impact. ^{233}U thermal and intermediate bare and water-reflected benchmarks agree well with ENDF/B-VIII.0. From ENDF/B-VIII.0 to ENDF/B-VIII.0b0.1, HMF-007 C/E are increasing and the new ^{19}F evaluation is helping the HMF-007 cases containing Teflon which have historically had high C/E. The Pu legacy benchmark suite is within experimental uncertainty with the exception of THOR. The INDEN evaluation followed by LANL gave the lowest mean absolute bias, but it remains difficult to make a determination on which Pu evaluation is the best. INDEN performs slightly better for the JEZEBEL series, while the LANL Pu evaluation is better for THOR and flattop benchmarks. For the PMI benchmark series INDEN outperforms the LLNL evaluation. For the PST benchmark series ENDF/B-VIII.0 and LLNL Pu evaluations are better than the INDEN evaluation. C/E ratios for Jezebel and Godiva reaction rate ratios show all the Pu evaluations are very close to one another, making it again difficult to say which is best. When examining neutron reactor kinetics parameters, each Pu evaluation is once again very close. Each individual Pu evaluation seems to have advantages in their own applications.

Discussion Items:

- **ACTION: Is there a possibility to merge different Pu evaluations?**
- **QUESTION**: Why is there negative sensitivity for the ^{239}Pu (n,2n) in LLNL Pu file?

        - Additional validation is needed to understand what is going on.
    - For the r5 model, the detailed and simple model average neutron energy causing fission differ by approximately 1%, why?
- **DISCUSSION**: New ^{19}F evaluation may improve benchmark performance.

ENDF/B-VIII.1beta0 Testing with LLNL Pulsed Spheres

Speaker: Denise Neudecker (Los Alamos National Laboratory, Theoretical Division)

Overview: Explore the use of LLNL pulsed sphere leakage (14 MeV D,T neutron spectra) input decks used to validate changes from ENDF/B-VIII.1b0.1a, to check elastic and inelastic cross sections as well as PFNS for fissile isotopes. Natural iron spheres (made up of 92% of ^{56}Fe) do not change for thin spheres and very slightly improve for thick spheres pointing to improvements in inelastic data at lower E_{inc}. Silicon spheres show no change between libraries for concrete (only 13% content). Thin ^{235}U (less than 1 mfp) improved due to new PFNS. These new PFNS data changed from VIII.0 based on new Chi-Nu data. Thick ^{235}U spheres have improvements and some decreased performance. Coupled with thin spheres, the ^{235}U spectra improved distinctly from 200-300 ns. There was little observable/contributable change to ^{238}U. For the ^{239}Pu performance, ENDF/B-VIII.0 is underpredicting for the valley of pulsed sphere in between elastic and inelastic peaks, other evaluations seem to improve. No clear winner can be distinguished between all four Pu evaluations (unknown characteristics of spheres also introduces uncertainty in measurements). Further development of forward versus rear facing detectors response need to be explored so the input decks can be matched to experimental results.

Discussion Items:

- **ACTION**:
    - TOF shift at certain angle is being investigated – efforts are underway to better understand pulsed sphere experimental data.

Contribution to the Validation of the INDEN Evaluated Data Files

Speaker: Andrej Trkov (Jozef Stefan Institute)

Overview: Fluorine, iron and copper were all tested. Issues in the ^{19}F inelastic cross section and elastic angular distributions were discovered. There are discrepancies when compared to the 1969 Broder experiment. Validation of Fluorine done primarily through HST benchmarks which are dependent on actinide RRR. It is recommended that a TSL evaluation be done for Oxyfluoride to more accurately simulate the benchmark experiments used for the validation of ^{19}F. Investigation and improvements to Cu have resulted in improvements to C/E of a suite of critical and subcritical benchmark experiments. Specifically, the INDEN evaluation performs very well in Cf neutron leakage experiment conducted at Rez. Unfortunately, efforts to reconstruct elastic scattering angular distributions from resonance parameters seem to have a negative impact on benchmarks. Further work is required to determine if this is a compensating effect from another portion of the evaluation. For the new Fe isotope evaluations present in INDEN, the Fe capture cross sections for energies below first resonance in ^{56}Fe have been reduced. INDEN evaluations of Fe also perform well on stainless steel reflected experiments and are within Rez benchmark uncertainty across the full neutron energy range. However, INDEN Fe evaluation does not improve high energy TIARA benchmark.

Discussion Items:

- **ACTION**:
  - More accurate fit to the broader data is planned for the future – fitting angular distributions is required.
  - Teflon TSL. Big discrepancies (40% in resonance spins?) in Ni LSDS spectra in the low-keV energy region.
  - Efforts needed to determine issues with Ni evaluation due to large contribution to issues in benchmark suite used for validation
  - Simple solutions are not the answer the final - f**ull re-evaluations are needed** to fully resolve discrepancies and make largest improvements
- **QUESTION**:
  - (Jesse Brown) PMI-002 is an outlier benchmark, what is the role of Ni in this benchmark? Was Nickle sample natural in LSDS?
    - Yes, it was natural
- **RESOLVED**:
  - Progress made in identifying nuclides/reactions that produce outliers
- **DISCUSSION**:
  - (Capote) There is unpublished new Cf neutron leakage in Ni showing that ENDF/B-VIII.0 is good, except from 1-2 MeV where a 20% underestimation is observed. Resonance benchmark is sensitive to neutrons above 1 MeV
  - LSDS data on Nickel looks very similar (Nick Thompson thesis work).
  - (Skip Kahler) Detailed simulation of PMI-002 with ENDF/B-VIII.0 is overpredicting (1.0196)
  - PMI002 has a very large transformation bias since it is an R/z – use the explicit 3D model for nuclear data testing. Detailed PMI-002 results is still roughly 2% high.
  - 1-2 MeV is very important and need to re-evaluate Ni to understand what is going on.
  - Rez benchmark document is available from INDEN webpage, but not available in ICSBEP benchmark just yet (aiming for spring 2023 release).
  - PMI-002 is extremely sensitive to Cr off by 2% compared to HMI001.

Preliminary fast benchmarking of 239Pu for ENDF/B-VIII.1

Speaker: Tim Gaines (AWE Plc)

Overview: Fast metal benchmarks were tested using new ^{239}Pu evaluations from ENDF/B-VIII.1 Beta 0, INDEN and LANL. The benchmarks of interest are in the PMF, HMF and MMF suites. The ^{239}Pu files p10, p17, p29, p39, p55, p56, Beta0 version a (p57), b (LANL), and c (ENDL) are processed locally using NJOY2016.67. The MCNP6 calculations are performed using inputs from the ICSBEP handbook. PMF021 has a significant increase in C/E for Beta0_c. A decrease is observed in PMF041 for all Pu evaluations. The INDEN evaluation underpredicts PMF-001 k_{eff} by a small margin. For MMF-007, Beta0_c stands out in the evaluation; however, the evaluations are in line with each other. INDEN ^{235}U and ^{238}U evaluations underpredict k_{eff} for Godiva (data processing discrepancies exist between sources of INDEN ACE files).

Discussion Items:

- **ACTION**

- Further investigation into the PMF-001 and HMF-001 calculations (discrepancies between self-processed and available INDEN ACE files (both using NJOY)).

- **QUESTION**
  - (For Mark Paris) will there be an update to Be in the next release?
    - *Response*: It is unclear if the file will be available for release for the next ENDF beta release, but there is a file available.
  - Are there any interesting MMF series benchmarks that are standing out/of interest?
    - *Response*: seems like MMF-007 is a Be reflected HEU with various reflectors and nothing is standing out too much.
- **DISCUSSION**
  - PMF-021 which sees a significant increase with Beta0_C PMF41 shows a significant decrease for all versions – needs attention.
  - (Capote) Nu_bar is increased everywhere by LLNL – main issue seen on slide 6 of 9. This may be due to the multiplicity changes.
  - (Skip Kahler) MMF-007 is "constant" Pu core with HEU then Be. HEU increases & Be decreases. Then a larger Pu core and repeat. Total of 5 different Pu cores and 23 total configurations. EALF varies from 0.064 MeV to ~1.0 MeV … so a nice suite to data test with.

Updated Gadolinium Validation in SCALE 6.3.0 using ENDF/B-VIII.0 Data

Speaker: William Marshall (Oak Ridge National Laboratory)

Overview: SCALE-6.2.2 showed a positive bias for k_{eff} resulting from an increasing concentration of Gd. Since there were few benchmarks with Gd available, the collection of Gd systems were expanded. All models used in Gd validation have been checked but are awaiting approval for VALID library. Many of the inputs have been developed as part of master's thesis or internships with US Naval Academy. All available input decks were run with SCALE 6.3.0 and ENDF/B-VIII.0 encompassing a suite of HST, LCT, HMT, MST, PST, etc. benchmarks. Summarizing, 6 existing benchmarks and 46 new configurations were tested, majority within 2 sigmas of uncertainties, few are above 3+ sigma. Looking across whole experimental range, the previously displayed positive bias rom Gd has been deemed no longer a trend and is probably a result of experimental biasing. HST benchmarks show largest variability, specifically HST-016 and HST-034. Conclusion, validation suite of gadolinium containing benchmarks has been increased by 99 cases. Misprediction and calculations observed over benchmark suite – but not systematic trends pertaining to Gd were observed.

Discussion Items:

- **ACTION**:
  - More experiments, consider more ICSBEP available Gd benchmarks.
- **QUESTION**:
  - Why is there no clear trend as a function of concentration or spectrum?
    - Same with solid absorber cases
- **RESOLVED**:
  - Finished the whole suite for ORNL VALID library (prev. Only HST-014 & HST-016).
  - 13 cases --> 99 cases. IPPE HST experiments completed.
- **DISCUSSION**:
  - Unreliable system geometries cause large variability in the C/E.

- LANL HMT experiments have significant discrepancies in Gd alloy cases.
- (Zerkle) Gd is very self-shielding, we need to understand microstructure of the Gd. Gd location and distribution is very important.
- (Dave Brown – Gustavo) Other changes were made in fission products (URR, thermal cross sections) - was Gd included? Beta will not include any changes to Gd at this time.

Recent Overview of the Fusion Evaluated Nuclear Data Library (FENDL)

Speaker: Tim Bohm (University of Wisconsin-Madison)

Overview: ^{19}F is very important in fusion applications, as molten salts (FLiBe) are proposed as a liquid blanket in fusion reactors. Calculations with this new evaluation show that the neutron flux increases between 20-70%, which indicates more shielding will be required. The FENDL-3.2 library is available on GitHub or the IAEA webpage. For some key isotopes (^{56}Fe, Cu, ^{52}Cr), the INDEN evaluation was chosen. Validation of the FENDL library was conducted using (D,T) pulsed spheres benchmark experiments. The JADE tool is also available on Git that allows automated validation testing of FENDL evaluations.

Discussion Items:

- **ACTION**:
  - A 'big paper' of FENDL3.2 will be submitted soon to Nuclear Data Sheets.
  - INDEN cross sections will continue to be investigated.
  - JADE may be moved to an open-source framework with the capability to utilize OpenMC, covariance data, etc.
  - Report data covariance matrices when they are available.
- **QUESTION**:
  - What is the physics of ^{19}F absorption that causes changes in the neutron flux?
    - ^{19}F inelastic was reduced which lowers absorption and will increase the flux above 1 MeV (where the largest changes were made).
  - (Nick Thompson) Would this higher flux also translate to higher shutdown dose rates?
    - *Response:* It would depend on the materials being activated, but most likely yes.
  - (Denise) What is the highest energy you will report covariances up to?
    - (Capote) we are in the start of the cycle of obtaining covariances, and we have a lot of data. This is not a very easy task and data covariances may not be available in the short-term. We provide data up to 60 MeV so the covariance will need to go up to 60 MeV as well.
  - (Andrej) Benchmark models are very high fidelity, and the transport of particles is intense, Monte Carlo is no longer really supported, need covariance to perform diffusion/reduced order modelling.
  - Why use ENDF/B-VII.I Cu and not INDEN?
    - (Capote) Cu has been evolving, at the time of release of FENDL3.2 there was not a final version of the Cu evaluation.
  - Does ^{19}F evaluation make things worse in specific energy regions in fusion reactors?
- **RESOLVED**:
  - Updates to FENDL (v 3.2b) 2/15/22 - 192 materials

- JADE automated validation tool is available.
- **DISCUSSION**:
  - There may be a need for more shielding behind the blanket region.

Status of ADVANCE CI/CD

Speaker: David Brown (NNDC, Brookhaven National Laboratory)

Overview: ADVANCE (automatically checking ENDF files as soon as they are released) is still down due to moving to GitLab. Interfacing with internal BNL clusters is problematic and collaboration with GitLab personnel will hopefully resolve the issue shortly. ADVANCE creates PDF summaries per push commit as replacement for the html pages generated. A brief demo for outputs generated from the checker codes was presented. It is very easy to run full on benchmarks in the Kubernetes framework will likely run OpenMC (but with a much smaller test suite), still need to discuss export controls.

Discussion Items:

- **ACTION**:
  - GitLab is complicated with national labs that need to work behind firewall – GitLab engineers working on this issue.
  - Generate a list that Dave Brown would like GitLab to do and have a meeting about this with all interested users.
- **QUESTION**:
  - (Nathan) is it easy to substitute in new checking codes if they were to become available?
    - *Response:* Yes.
  - (Zerkle) Will this include all sublibraries?
    - *Response:* yes, but not all sublibraries will have the same set of checking codes running.
- **RESOLVED**:
  - Simpler PDF reports are now generated on a per commit bases.
- **DISCUSSION**:
  - Waiting on BNL server implementation.

Status of ENDF Reviews

Speaker: Gustavo Nobre (BNL)

Overview: ENDF/B-VIII.1 will be released in 2024. ENDF/B-VIII.beta1 release scheduled for December 2022. There will be multiple sub releases because of the amount of work and updates relating to ^{239}Pu , ^{235}U and ^{238}U. ^{19}F, ^{56}Fe, and ^{239}Pu all changed from ENDF/B-VIII.IBeta0.1 to ENDF/B-VIII.I Beta0.2. Verification and validation of actinides in ongoing review process for ENDF/B-VIII.1. ^{16}O, ^{18}O, ^{10}B, and ^{11}B are not ready for submission. ^{50,52,53,54}Cr evaluations have all been approved. Number of TSL evaluations are on track to double! Significant additions made to alpha, deuteron, decay, fission yield, and photonuclear sub libraries.

Discussion Items:

- **ACTION**:

    - Plan another hackathon or mini-CSEWG in the near future
    - CSEWG executive committee needs to decide best course of action towards Beta1
    - Collaborative review of new TSL sub-library submissions
        - Create new platform for the ease of this review between collaborators
    - Push fission yields forward
    - Bottleneck is currently **REVIEWERS** – looking for volunteers
        - (Devin Barry) Need feedback from reviewers on how to best complete this process
- **QUESTION**:
    - (Jesse Brown) Will all submissions be included in next beta/is beta1 a complete release?
        - *Response:* Yes, timeline is proportional to number of reviewers
- **RESOLVED**:
    - The hackathon was productive in discovering and resolving issues in current evaluations
- **DISCUSSION**:
    - TSL – plan to use NCSU internal review approach

Calculation parameters vs data in burnup calculations

Speaker: Andrej Trkov (Jozef Stefan Institute)

Overview: A sensitivity analysis using multiple nuclear data libraries, codes and burnup parameters on a 3x3 PWR assembly was performed with a focus on fission yield interpolation. The test case observables are isotopic concentrations, absolute reactivity, and normalized reactivity at 500 MWD/MT-HM. Serpent and OpenMC can produce (almost) identical results when adjusted. Currently in ENDF/B-VIII.0, fission yields are provided for thermal, epithermal, and fast energies. While not physically correct, Serpent obeys linear interpolation while OpenMC uses thermal yields. There are little to no observable differences in absolute short burnups. Renormalized reactivity shows slight systematic dependence on the Q-values used for the calculation. ENDF/B-VIII.0 library yields a steeper reactivity burnup profile in Serpent using default settings (and comparable OpenMC) calculations with PWR fuel, compared to the ENDF/B-VII.1 library burnup parameters, models and data all have strong effects on reactivity burnup profile. Energy deposition parameters AND library effects on the reactivity burnup profile must be considered when evaluating library performance for real reactor systems. Burnup in PIE benchmarks can be normalized to burnup monitors; this is not possible for operating reactors (e.g. cycle length comparison)

Discussion Items:

- **QUESTION**
    - (Chadwick) - Were differences between ENDF/B-7.1 and ENDF/B-8.0 in fission yields a result of fission product energy release difference between the evaluations?
        - *Response*: Further investigation would be required to be able to attribute this discrepancy to a particular difference between the evaluations (for example assumptions in SERPENT can influence how data is ultimately used).
- **DISCUSSION**

- Inclusion of other interpolation options in Serpent (currently based on neutron energy spectrum)
- ENDF/B-VIII.0 has issues with production gammas (NNL testing – Zerkle) energy release per fission product

Evaluation Committee [Neutrons]

Chair: Mark Chadwick (LANL)
Date: Tuesday, November 1, 2022

Welcome and comments

Speaker: Dave Brown (BNL)

Overview: Welcome! Day 3 of CWESG (tomorrow) is in the Physics building.

Evaluation session opening comments

Speaker: Mark Chadwick (LANL)

Overview: Welcome! Lots of interest exists in new evaluations coming in down the pipeline.

Chadwick adds: ^{239}Pu in the fast range was not described in great detail at the main CSEWG meeting, since a previous meeting focused on the various fast region evaluations: the INDEN (ORNL-IAEA-LANL) and the T2/LANL one. At the Tuesday Exec Committee meeting it was decided that beta1 fast region would be a hybrid merged file, with elastic and inelastic coming from T2/LANL and n,2n and capture from INDEN. Kawano indicated that their new n2n is supported by the individual gamma-rays from GEANIE – we agreed to study this in the coming months, because it is not desirable to reduce n2n at 14.1 below the accurate (activation data) Lougheed (McNabb) error bars unless there is a strong compelling reason. A new merged beta1 starting file was created by the IAEA, and after more resonance work is done with ORNL it will be released in beta (target date end of Jan 2023).

Summary of ENDF library work

Speaker: Gustavo Nobre (BNL)

Overview: There is a lot of great work being done at the NNDC, who will be hosting another hackathon and mini-CSEWG between the releases of ENDF/B-VIII.1b1 and ENDF/B-VIII.1b2. Work is being done to improve the reproducibility of evaluations, which will make it much easier to incorporate improvements into said evaluations. Gamma spectra are being revised during evaluations, and do not preserve what is currently present in the ENDF/B-VIII.0 library. Evaluators need to be mindful to track the history of their files in all phases of the evaluation in each branch (phase 2/3, etc.). The NNDC is actively looking for volunteers to review evaluations.

Discussion Items:

- **ACTION**:
  - Schedule another ENDF hackathon for 2023.
  - CSEWG executive committee needs to decide best course of action for Pu evaluation for ENDF/B-VIII.0b1.

    - Gamma spectra should be improved consistently with the rest of the evaluation (instead of overwriting/ignoring existing information/not formatting the spectra).
    - **Get volunteer reviewers: especially for the decay, fission and neutron evaluations**
    - Need to move fast to review evaluations that have been submitted for the release of ENDF/B-VIII.0b1
- **QUESTION**:
    - (M. Herman) SG49 is tackling the evaluation reproducibility problem – will you be able to contribute to this subgroup?
        - *Response:* Yes.
    - (Denise) Will evaluation changes and information be stored in the trackers?
        - (Gustavo) we haven't thought about this because no one submits this information at this time.
        - (Dave) We collect LEAPR and other files in the TSL sub-library, we can start doing this with other sub-libraries.
        - (Doro) there should be an agreement on the format this information will be provided in (I.e. GNDS).
    - It would be nice if level energies in ENSDF and ENDF were in agreement with each other.
        - *Response*: Of course. If they are well-known, this is something that should be pursued.
    - (Trkov) Files are often iterated upon one another, so the entire history of changes should be stored – which makes the process cumbersome.
        - (Gustavo) An assembly script should be built to store the detailed history of the evaluation in order to preserve the full history of the evaluation.
    - Git can only store so much information – files that are intermediate should not be stored.
        - Virtual environments may provide a guarantee all evaluation codes will work as intended
- **RESOLVED**:
    - Many isotopes have been approved for submission into ENDF/B-VIII.1b1.
- **DISCUSSION**:
    - Gustavo's wish on evaluation reproducibility:
        - Evaluations should include all information about how files were produced.
            - Most ideal – virtual environment with all evaluation and assembly codes and inputs, where evaluation can be reproduced with a single command.
        - There are different levels of how to do this: detailed, quantified, well-documented description of what was done, portable script that does the file assembly

INDEN Si, Cr, Fe, Cu, U, F isotopes

Speaker: Roberto Capote (IAEA NDS)

Overview: The INDEN collaboration has produced many new evaluations for various elements, including Si, Cr, Fe, Cu, U, and F. Integral data suggests that there are problems with existing nuclear data so new experimental data is always required. The Curie benchmarks are shown to be very sensitive

to Cu and ^{19}F and are overpredicting k_{eff} by >1000 pcm with the new INDEN evaluations of ^{56}Fe and ^{19}F. ^{19}F inelastic scattering data and elastic scattering angular distributions are in great need of new measurements and evaluations. The elastic scattering cross section for ^{19}F was reduced by 40% in the INDEN evaluation around 300 keV. Additionally, there are large issues seen in Cu, based on Cf-leakage experiments conducted at Rez. The ENDF/B-VIII.0 elastic cross sections for Cu are low compared to JENDL-4.0, so there was a need to renormalize the elastic cross section while keep the total the same. The ^{63}Cu capture cross section was changed to agree with Los Alamos Weigand and Newsome experiments below 1 MeV. ^{56}Fe was also shown to underestimate neutron leakage between 1-4 MeV and overestimate the neutron leakage around 1 MeV from a similar Cf leakage experiment. Based on thick-sample transmission measurements conducted at nELBE, the ^{57}Fe cross section was then changed to fill in the minima in the ^{56}Fe cross section. The ^{57}Fe RRR was also extended based on total cross section data available from Pandey. The ENDF/B-VIII.0 ^{181}Ta evaluation disagrees with some capture experimental data from 1-2.5 MeV. The new copper 63, 65 evaluations now well represent the dosimetry reactions for each isotope.

Discussion Items:

- **ACTION**:
  - ^{63}Cu(n, g) and ^{63}Cu(n, α) measurements/evaluation work may be needed.
  - More inelastic scattering data for ^{19}F.
  - Reach out to Morgan to discuss work on gamma ray data (glmorgan@lanl.gov).
- **QUESTION**:
  - (Denise) Will there be reported covariance?
    - *Response*: These are older data, and based on limited time, considering and reporting covariances are difficult.
- **RESOLVED**:
  - New transmission measurement at nELBE (thick target) - ^{56}Fe
    - Determined the issue is in the ^{57}Fe evaluation – which was changed to fill in the ^{56}Fe minima.

RRR for ^{233,235}U and ^{239}Pu

Speaker: Marco Pigni (ORNL)

Overview: Issues regarding the actinides have been found in ENDF/B-VIII.0 evaluation(s) due to misprediction of some critical experiments. For ^{233}U, reactivity for critical assemblies was underestimated so there have been updates made to the PFNS, thermal constants, and R-matrix parameters which improves a subset of benchmarks. The RRR was extended up to 2.5 keV and validation with 180 benchmarks showed an increased reactivity trend. For ^{235}U, reactivity rates related to depletion calculations need to be investigated. Improvements of low reactivity at high burnup are needed so Wallner sub-thermal data are being evaluated. Bound resonances were tweaked to address capture/fission ratios to match the new measurement. For ^{239}Pu, the latest ENDF file up to 5 keV is released and actively being tested, validated, and verified. Mosby capture-to-fission ratio data are being included in this evaluation. Some work is still being done to tweak resolution functions in SAMMY to include some broadening seen on the lower tail of some resonances. Preliminary covariances may be provided by January of 2023.

Discussion Items:

- **ACTION**:
  - Sub-thermal ^{235}U data measured at HZDT needs to be considered
  - Determination of resolved and unresolved resonance parameters for neutron multiplicities of ^{233}U is needed.
- **QUESTION**:
  - (Skip Kahler) Is the 5 keV RRR extension work in all three candidate ^{239}Pu files we've been testing in e81b0abc?
    - (Capote): No, the extended RRR is not yet in ^{239}Pu files. we were conservative.
  - (Denise) Wondering about fluctuations in ^{233}U PFNS?
    - *Response*: Looking at available experiments of the PFNS.
  - (Capote) you mentioned alpha Mosby and we know they need to be correlated so are you considering this?
    - *Response:* Yes, that's what I want and I'm excited to get data to see the consistency – capture and fission.
  - (Talou) Could you comment on the need for new precise measurements of nu-bar fluctuations for those isotopes? There is also the question of feasibility to experimentalists…
    - *Response:* Spoke with Kraft about a neutron multiplicity measurement and it is not an easy experiment but open to discussion.
    - (Capote) The last attempt was made at Geel. It is hard to get statistics these days. They used larger samples in the old times.
      - (Talou) Are you referring to Hambsch's measurements? We certainly need better data, but I understand it's tricky. Looking beyond just nu-bar is probably the way to go. We need to measure the gammas in coincidence, and possibly the fragments TKE.
      - (Capote) Yes. ^{235}U measurements. Nobody tried to measure Pu for a long time, nor ^{233}U.
  - (Chadwick) How is ^{233}U and Th performance in benchmarks? Pu evaluation accommodated a softer PFNS – has that changed at all?
    - ^{233}U – we need to focus on the poorly performing benchmarks.
    - Pu – deeper analysis is required for the thermal point and the first few resonances.
    - Zerkle – Use UCT-001/UCT-004/HCT-015 - LWSB experiments with ^{233}U seed + blanket.
      - Solution criticals are not trustworthy because we do not know the solution chemistry.
- **RESOLVED**:
  - Pu evaluated resonance parameters and related covariance matrix were adopted from WPEC (SG-34)

Evaluation and validation of ^{63,65}Cu

Speaker: Jordan McDonnell (UT-Battelle)

Overview: There was an update to ^{63,65}Cu cross section evaluations using recently measured data to resolve discrepancies in the performance of benchmarks. The primary challenge in the RRR was to resolve the discrepancy between available measurements for ^{63}Cu(n,g). There is a high-resolution capture measurement from GELINA (Guber, 2014), which has a lower capture yield above 20 keV than the lower resolution LANL measurements (Weigand, 2017). In this work, the Guber measurements were normalized above 20 keV by a factor of 20% to improve alignment with Weigand's measurements. Past work has demonstrated that the criticality benchmarks are very sensitive to ^{63,65}Cu ESADs. The ENDF/B-VIII.0 Legendre coefficients exhibit a discontinuity at the transition from the RRR to the fast region. Legendre coefficients from experimental measurements by Popov (1986) and Smith (1967) are adopted from 100 keV to 1 MeV for both isotopes. Data is unavailable for R-matrix analysis above 100 keV. In the fast region, ENDF/B-VIII.0 cross section agree well with measurements up to 4 MeV, but deviate above 4 MeV. The JENDL-4.0 cross section agree with measurements above 4 MeV. Adopting the JENDL-4.0 above 4.0 MeV improves performance in the Rez shielding benchmark. The evaluation of this work leads to improved agreement between measured and calculated k_{eff} in ICSBEP criticality experiments. The adjustment to the Legendre coefficients contributes to overall agreement, and the increase in the ^{63}Cu capture cross section reduces the trend in the ZEUS (HMI-006) series with respect to EALF. The ^{63,65}Cu cross sections have been updated to 100 keV.

Discussion Items:

- **ACTION**:
  - Additional tweaking to improve benchmarks that are not performing well.
  - Resolve discrepancy in Rez Cf-neutron leakage experiment below 100 keV.
- **QUESTION**:
  - (Roberto) The hmi006 Zeus improvement is due to Cu but also due to a change in ^{235}U nubar.
  - (Dave Brown & Zerkle) Some benchmarks perform well but others don't - still needs tweaking.
  - (Yaron Danon) Was a comparison made to the quasi-differential data for the angular distributions?
    - *Response*: Yes, the changes improve the discrepancies seen in those data, not shown in slides.
  - (Bob Little) I think you said that the angular distributions < 100 keV were from resonance parameters. Are these using the explicit format formalism that indicates "reconstruct angular distributions from resonance parameters" or are these some sort of smooth fits with actual Legendre parameters given?
    - *Response:* They are not using format formalism – used SAMMY to construct the angular distribution from resonance parameters.
    - (Roberto) There is still a discrepancy in the pulsed data below 100 keV.
- **RESOLVED**:
  - ^{63,65}Cu cross sections have been updated to 100 keV.
  - JENDL-4.0 cross sections adopted > 4 MeV for agreement with Rez neutron leakage experiments.

Secondary distributions added to file

Speaker: Hye Young Lee (LANL), Ian Thompson (LLNL)

Overview: (Two-part talk)

First part from Ian Thompson:
Exit distributions for photon and charged particles missing from ENDF/B-VIII.0 have been added. There are still missing exit distributions leading some transport codes to fail, so this work proposes to transplant distributions from TENDL2019. There are currently no sources for some light (Z<10) targets will with need some R-matrix evaluations. In conclusion, LANL has better distributions to add for exit p, α. Some exit distributions may be improved by the GRIN project.

Second Part: Hye Young Lee:
Deficiencies in simulated charged particles are seen when compared against measured from LENZ data. New evaluation using new ^{54}Fe data can be completed using a partial update or a new evaluation. A partial update would include re-evaluation for only (n,n') and (n,np) cross sections and reconstructing other channels. A new evaluation can be done using model parameterizations and by reproducing all channels carefully. Currently, Empire and CoH3 are used with CCOMP adjusted OMP from Spherical Koning local OMP (RIPL ID. 1414) CC (2 = 0.15) calculation with DWBA. Production cross section that was measured at 53 degrees was compared with the new evaluation ("present"), ENDF, and JENDL. There is also new LENZ data on stable Ni, where a new evaluation is still in progress. ^{54}Fe inelastic was changed based on the Olacel 2018 data, (n, np), (n,Xα) were also changed slightly. There is a need to separate the cross-section data into respective files, cross section in MF3, energy-angle in MF6, angles in MF4, and Photoproduction in MF14. To accommodate file sizes, all reaction channel excited states should be kept to 10 max.

Discussion Items:

- **ACTION**:
  - (Part 2) Hye Young Lee
    - Plans for secondary distribution for ENDF/B-VIII.1
      - There is a collaboration with LLNL and BNL for merging both efforts into the new ENDF release (making decisions on how to consistently merge the secondary distribution files over a broad range of nuclei, expect the energy balances for those channels will be improved with this effort)
      - LANL-KAERI plans to complete new evaluation based on new experimental LENZ data of ^{54}Fe, ^{56}Fe and ^{58}Ni, ^{60}Ni (will update cross sections for (n,p) MT=103, (n,np) MT=28, (n,d) MT=104, (n, α) MT=107, and (n,nα) MT=22 and differential cross sections of discrete states for protons in MT=600-609 and α's in MT=800-809)
- **QUESTION**:
  - (Part 1) Ian Thompson
    - (Caleb Matoon) Will the thresholds need tweaking?
      - *Response:* Yes.
    - (Chadwick) Does it run on Livermore codes? MCNP?
      - (Bob Little) MCNP makes some assumptions in order to do the transport. Local deposition of energies, checking energy balances, etc.

        - (Mike Herman) There is a small miss in the format. Internal electron conversion cannot be handled, need to either put it into gammas and overshoot or put into Qrxn and calculate 3-4% lower. If we put it into the evaluation with gammas, the calculations are correct and lower energy transition to the ground state does not produce gammas which could be slight overestimation so we need to document this correctly.
    - (Part 2) Hye Young Lee
        - (Gustavo) What will be done to merge this evaluation?
            - Multiple layers and hierarchy of merging and decision making will be needed.
        - (Chadwick) Old measurements exist, how consistent are those results with your work?
            - These measurements are in fairly good agreement with some measurements that were taken straight from EXFOR.

^{181}Ta

Speaker: Mike Herman (LANL)

Overview: There is work to constrain the ^{181}Ta(n,g) reaction with available data. The fast region calculations are done with an energy dependent normalization (primarily McDermott & Dsyziuk data). Capture gamma spectra are also reproduced well; there is a high energy tail related directly to capture which may suggest capture at a few MeV may be higher. ^{181}Ta(n,2n) is now in better agreement with two selected experiments by changing the level density in the target nucleus. Major disagreements are still in the inelastic cross section: the 1st inelastic state is lower than Rogers data, while higher inelastic states have better agreement. For the total cross section, spherical optical model over-calculates below 0.7 MeV. This work and JENDL-5 are both very similar to one another, but different choices have been made for the inelastic and capture cross section. The file has been merged with the NNL/ORNL RRR evaluation. Performance of this evaluation work is improving on validation benchmarks (PMF-045 + new TeX-Ta benchmark experiments).

Discussion Items:

- **ACTION**:
    - New ^{239}Pu evaluation should be taken into account with TeX validation.
    - **EXFOR files (Rogers Ta inelastic xs?) need to be marked as theoretical calculations and not as an experiment.**
    - Possibly put more structure into evaluation.
- **QUESTION**:
    - (Gregory Potel) Isn't there a concern about changing a parameter (say, level density) for one channel (say, n2n) without checking how it will affect others? How does one restore consistency?
        - *Response*: If you change it – there will be a reflection in other values.
    - (Marco) Do you think that the EXFOR data needs to be corrected?
        - *Response*: Experiments are taken from EXFOR as is. This should be corrected in EXFOR. Unsure how JENDL is high, cannot explain difference.
        - (Chadwick) when there is an error in EXFOR, can the files be removed?

        - *Response:* Should be marked there is an error but everyone says "no" to removing it completely.
        - Emphasis placed on needing to make sure the mistake does not happen again.
    - (Denise) Excited for covariances – is Marco also doing this?
        - Covariances from Marco are available.
    - (Chadwick) Yaron is sending tungsten data – is there also Ta scattering?
        - (Danon) can't remember but doesn't think so – did we give you total in the fast region (0.5-20 MeV)?
            - *Response:* (Mike Herman) took it, smoothed it and cut off lower points.
            - (Danon) there's lots of structure up to 2-3 MeV.
        - (Zerkle) There is an opportunity to measure Ta and Teflon.
- **RESOLVED**:
    - Ta(n,2n) cross section is now in better agreement with experimental data.
    - Evaluation file merged with the new NNL/ORNL Resonance Region and submitted to the NNDC Git repository with preliminary covariances (by January).
- **DISCUSSION**
    - (Wim Haeck) for the ZPR plates, less ^{239}Pu than expected in the experiment than in benchmark calculations is shown to shift 50-100 pcm down.
    - (Capote) important to see that there are theoretical values in EXFOR that are not experimental – also, (n,2n) outliers in data can be corrected.
    - (Capote) we should aim at getting mean values consistent with covariances. You can only enforce that if you adopt the GLSQ fit for the mean values as well. You do the GLSQ with your selected measurements

Pb isotopes

Speaker: Peter Brain (RPI)

Overview: There is a growing need for accurate lead evaluations for lead fast reactor concepts and new accelerators which will utilize lead. Pre-evaluation showed that elastic scattering angular distributions and the RRR of ^{206,207,208}Pb were major areas of disagreement between international evaluations. To resolve angular distributions issues, quasi-differential data scattering data measured at RPI were used to constrain the evaluation. An iterative process was created using SAMMY, NJOY (Blatt - Biedenharn), and MCNP to determine resonance parameters above current ENDF/B-VIII.0 evaluations. The LANL ^{208}Pb fast evaluation from T. Kawano was merged into the RPI ^{208}Pb RRR evaluation to create full energy spectra evaluation. ^{206}Pb evaluation now includes more total cross section data in the form of distribution through inelastic channels. The RPI evaluations now predict current fast benchmarks very well, but this is difficult to attribute solely to Pb due to potential compensating effects in the benchmarks.

Discussion Items:

- **ACTION**:
    - ^{208}Pb drives anisotropy in quasi-differential scattering data so a re-evaluation is needed to make RRR or ESAD improvements.
    - ^{206}Pb fast region evaluation is needed.

- Covariance development is necessary for all energies.
- A compensating isotope that might be causing discrepancies in benchmarks, so this needs to be investigated.
- Submission of Pb evaluation work up to this point should be included in Beta1 without covariances so it can at least start getting reviewed.

- **QUESTION**:
  - (Denise) Do you fix the number of resonances you sample when you randomly sample?
    - *Response:* The random sampling is done on a per resonance basis.
  - (Gustavo) When is this going to be submitted to NNDC?
    - *Response:* Submit to Beta1 ASAP without covariance and submit finalized with covariance to Beta2

- **RESOLVED**
  - 50 p/d-wave capture resonances added in ^{206}Pb.
  - Elastic scattering angular distribution and resonance parameter scheme were both automated, which leads to major improvements when comparing to the RPI scattering data.
  - T. Kawano's fast region evaluation was merged above 2.5 MeV with RPI evaluation below 2.5 MeV.

n+^{16}O & Charged-particle sublibrary evaluations in multi-channel unitary R-matrix approach

Speaker: Mark Paris (LANL T-2)

Overview: ^{16}O evaluation updates are coming with ENDF/B-VIII.0b1, where the (n,α) cross section is set by Bair & Hass (1973) data that are good to 10% of the original normalization value. There may be too much absorption for fast critical benchmarks. (α, n) to (n, α) were set with Perchenko data, which are in agreement with evaluations and cross sections. There are currently no changes as a result of rescaling partial channels in the (n, α) or excited states. There is currently very little change observed in critical experiments with no improvement or harm done.

Discussion Items:

- **ACTION**:
  - Discuss with Capote regarding the changes in ^{16}O and ensure that there are not any changes in the total cross section.
- **QUESTION**:
  - (Chadwick) Should we put this update into Beta1?
    - *Response:* More testing with the file is most welcome but if there is no change then stick with the previous version
    - (Chadwick) But if you corrected it and think there is reason for that – should this update be included?
    - (Paris) Still worried about the Davis data. Chadwick adds, per an email discussion with Paris, Paris agrees that this version – worked on a bit by Capote too - will go into beta1 (unless some further update is produced very quickly and is tested and viewed as attractive for release by end of Jan 2023).
  - (Capote) Did you compare the changes in the total to experimental data?

        - *Response:* Changed inelastic, not the total (total was maintained because there is accurate data, i.e., Cierjacks 1980)
        - Above 7.5-8 MeV, some argument to be made that we don't know gs contribution as well as we may think
    - (Yaron) Was the EXFOR experiment re-normalized?
        - Gerry says we did make the 3% correction needed to the EXFOR experiment.
    - (Klaus) In reference to the Cierjacks data there is a resonance seen in the experiment but isn't in the ^{16}O cross section, where is this from?
        - We will look into this, there is no clear answer at this time.
- **RESOLVED**:
    - Khryachove & Prusachencko 2022 have been updated (n, α_0)
    - Recommendation: Stick with ENDF/B-VIII.0 until further testing and work is done.
- **DISCUSSION**:
    - (Zerkle) There are usually compensating errors so seeing no harm done in benchmarks with the evaluation is very encouraging.

^{235}U PFNS and nubar and ^{238}U nubar work in progress

Speaker: Denise Neudecker (Los Alamos National Laboratory)

Overview: LANL is performing an evaluation of the ^{235}U and ^{238}U nu-bars and ^{235}U PFNS with new experimental data with improved experimental UQ and CGMF as input. The codes used were ARIADNE and CGMF with Kalman including correction for PPP evaluation technique. Evaluated ^{235}U nu-bar, with and without CGMF, is very similar to ENDF/B-VIII.0, but a tweak could be needed from 3-5 MeV. ^{238}U nu-bar is very different from ENDF8.0 from 2-4 MeV, because differential experimental data were not fully analyzed for ENDF/B-VIII.0. There, is a question whether Frehaut (lower) is right or Nurpeisov or Vorobyeva data (high), Sabin is somewhere in the middle. It is unclear which experiment is right given the high quality of all four. FF angular distributions could play a role to lead to bias there. So, there is a need to look at compensations between nubar and PFNS. Chi-Nu data is expected to come FY23 and expect nu-bar will be measured by the CEA. Nu-bar changes below 2 MeV are minimal, but above 2 MeV some differences begin to emerge due to the inclusion of more datasets in the evaluations. The recommendation is to not include in this in ENDF/B-VIII.1 until experimental data is confirmed. There is also a need to counterbalance change in nu-bar by PFNS. For both ^{235,238}U, the evaluated parameters link favorably back to other fission quantities, except for PFNS, using CGMF. Using CGMF for evaluations brings the added benefit that we can link back nu-bar to fission product yields, TKE, etc. to see if they are all consistent and realistic. More validation cases will be needed to validate the results of the new evaluation based on new Chi-Nu data.

Discussion Items:

- **ACTION**:
    - Work at LANL will focus now on understanding ^{238}U(n,f) nu-bar, PFNS will be updated in the next few months based on CEA and/or Chi-Nu experimental data.
- **QUESTION**:
    - (Chadwick) Is CEA going to use the PFNS to estimate nu-bar?
        - *Response*: Yes, uncertainties should be reasonable.

- (Capote) Angular distribution might have a different input compared to PFNS experiments? Should we check different experiments?
  - *Response*: There are no new techniques so that is not the issue and we are unsure which one is right.
  - (Capote) seen something similar for ^{232}Th (?)
- (Chadwik) In the case of ^{235}U nu bar, there is a difference in pure data and calculation approach in 3-5 MeV. I also see a deviation starting at 0.2 MeV?
  - *Response*: ENDF/B-VIII.1 starts at 0.2 MeV, ENDF/B-VIII.0 was used below to take a conservative approach.

- **RESOLVED**:
  - ^{239}Pu/U PFNS at 1.5 MeV looks good
  - Improved nuclear data for the ^{235}U PFNS and nubar in ENDF/B-VIII.1.

Photonuclear evaluation perspectives

Speaker: Mark Chadwick (LANL)

Overview: ENDF7 uses a large collection of photonuclear data, many from LANL and some from IAEA. Many DOE applications exist from photonuclear data. IAEA photonuclear libraries were updated, but limited US evaluations were submitted. For the coming ENDF/B-VIII.I release, we need to decide whether to adopt IAEA files or create new evaluations. Validation to follow.

Discussion Items:

- **ACTION**
  - Decide whether to adopt IAEA files or create new evaluations
- **QUESTION**:
  - (Yaron) In these files there are angular distributions that cannot be used in MCNP and NJOY.
    - *Response*: that's been fixed in NJOY and in MCNP6.3 (unreleased)
  - (Capote) new IAEA library calculation of (g,n) is underestimated because we did not pay enough attention near the threshold - fission gamma spectrum
    - *Response:* Fission gammas are a missing component, LANL has worked on new fission gamma spectra and multiplicities (but this is different from what Capote is asking about)
    - (Wim) we care about actinides, bremsstrahlung targets, Be, bremsstrahlung spectrum for accelerator applications – lower energies (5-8 MeV) photonuclear comes up here so it matters how we rise from threshold (user perspective)
- **DISCUSSION**:
  - New file? Can be demonstrated to be better & tested adequately
    - Is it a good idea to adopt a foreign file from IAEA?
    - Need to compare cross sections and test in MCNP applications
    - Chadwick noted that the IAEA CRP evaluations most likely are worth adopting, but we need to see case-by case comparisons of g,1n,2n,f,xn, etc of proposed v B8.0 v data, especially for important application nuclides

(actinides, bremsstrahlung conversion targets, structural and shielding nuclides, neutron sources like (Be, D), biological elements).

Preliminary look at IAEA photonuclear

Speaker: Wim Haeck (LANL)

Overview: Up to this point, the processing and validation of photonuclear data has been limited. The LA150U and ENDF70U are the only libraries available, and there is a need for new photonuclear ACE library for ENDF/B-VIII.1. At this time, only MCNP6.3 is capable of using the photonuclear ACE files produced by NJOY2016.66. Various validation exercises have been conducted using MCNP6.3 for the photonuclear data. There are currently only Barber and George (1959) measurements available to validate cross section data, attempting to use these results in MCNP giving some non-physical energies, indicating either an evaluation or MCNP issue.

Discussion Items:

- **ACTION**:
  - Produce a new photonuclear library ACE library based on ENDF7.1
  - Work needed in NJOY for corrected evaluations
  - Update made to NJOY2016.66 to allow for anisotropy in secondary photon distributions (fixed ACER module)
  - Looking for any type of experimental data for validation
- **QUESTION**:
  - (Capote) Al issue is corrected and you can download it from IAEA webpage
  - (Jason Thompson) Can NJOY process the resolved resonance region for photonuclear data?
    - *Response:* Work for Be is being done.
    - Photonuclear resonance parameters exist from Jason Thompson; Wim will follow up with him.
  - (Dan Roubtsov) - Laboratory frame of reference/CoM is broken in photo-nuclear evaluations and results in weird averaging of outgoing energy/masses.
    - *Response:* we need a verification step FIRST as the library is full of surprises.
    - Simple tests need to be conducted for all ACE files to confirm that simple physics are satisfied.
- **DISCUSSION**:
  - (Gustavo) Phase 1 can create individual merge requests for experts to look at it and verify what makes sense to accept/reject

Evaluation Committee [Thermal Neutron Scattering]

Chair: Ayman Hawari (NCSU)
Date: Tuesday, November 1, 2022

Neutron Pulsed Die-Away Experiments at LLNL

Speaker: Ruby Araj (LLNL)

Overview: Pulsed neutron die-away (PNDA) experiments were conducted at LLNL to validate absorption and scattering cross sections of the target medium. Low experimental uncertainties are possible without the need for fissile material in PNDA experiments. A DT neutron source is used to generate 14 MeV neutrons and the exponential decay of neutrons is measured with ^{3}He neutron detector. A combination of HDPE+Cd are used to shield the system from room return effects. The shielding box used in the PNDA experiments has its own exponential decay profile which must be accounted for. Small targets (large bucklings) are more sensitive to scattering and large targets (small bucklings) are more sensitive to absorption. Good agreement in absorption cross section in LLNL experiments is observed when compared to Nassar & Murphy and Bracci & Coceva data. The general trend is increasing bias with smaller sampler size (larger buckling) for HDPE and Lucite. PNDA experiments offer a great way to validate cross sections and TSLs.

Discussion Items:

- **ACTION**:
  - Fully characterize source, potential effects, other experimental considerations
  - ^{6}Li and ^{10}B target measurements
- **QUESTION**:
  - (Jesse Holmes) Is there a comparison to previous experimental data?
    - *Response*: Differences at higher buckling could be due to poor TSL evaluations because of higher sensitivity to TSL.
  - Why is a DT source used?
    - *Response:* While higher energy (14 MeV) neutrons are not desired, the high intensity of a DT source is optimal to obtain lowest uncertainties in experimental results.
  - (Hawari) if you have a 10 us pulse width, when do neutrons get to the thermal range (for hydrogenous samples especially)?
    - *Response:* The effect of the pulse width and the time it takes for a neutron to thermalized in a hydrogenous moderator can easily be calculated (between 0.5 and 2.0 ms).
      - (Hawari) thinks this is too long – follow up
  - (Trkov) It was said that you need a source of high energy but you are testing TSL models. How does this go together?
    - (Jesse Holmes) High-energy neutrons are thermalized via downscattering. When thermal and spatial equilibrium is reached, then counting begins to determine the characteristic decay time eigenvalue. High-energy neutrons are not "needed," but they are what you get from a D-T source.

NeTS Modules for Graphite and Beryllium

Speaker: Jonathan Crozier (NCSU)

Overview: Motivation for this work includes developing a compact formulation for TSL data which extends A.I. knowledge in the advanced reactor simulation framework. Neural networks are being explored to accurately represent continuous energy TSL nuclear data with a much smaller footprint than the current MF7. Graphite and Beryllium metals were chosen as materials to test A.I. approach due to wide variety of material complexity from both grain boundary and inter-atom bonding. Transform alpha, beta, and temperature to bound a smaller design space to train against. The number of layers and layers per node were evaluated to test the true 'weight' of the neural network. The neural network design that worked optimally for Graphite did not work with Be metal and vice versa. There was a need to optimize the hyperparameters within the model, and more work is needed to expand encompassing of model to include porosity, burnup, pressure, new materials. This approach is interpolation free and gets around the need for lookup tables needed to bound desired temperatures.

Discussion Items:

- **ACTION**:
  - Optimization of the overall neural network is required to reduce the network size, training time, and overall computational footprint.
    - Include one-phonon correction and train highly structured S(α,β,T) surface
    - Extend dimensionality: additional properties (i.e., porosity, burnup, pressure), new materials, extreme temperatures (cryogenic, advanced reactor conditions)
    - Couple NeTS to reactor physics framework
  - Include one phonon correction on highly trained 3D S(α,β,T) models
  - Coupling with codes
- **QUESTION**:
  - (Amber Coles) What neural network package was used?
    - *Response:* PyTorch
  - (Danon) Have you tried different activation functions?
    - *Response:* Leaky ReLu activation function seems to work the best, the activation function was played with.
  - (Danon) Lookup Tables vs NETs – how do the performance compare?
    - *Response:* Not in a framework yet. On the fly temperature reference is fast.
  - (Devin Barry) Is the current NN overfitting the data due to the multiple hidden layers?
    - *Response*: Overfitting is not a problem due to inherit data complexity.

Update on NNL TSL Evaluations

Speaker: Jonathan Wormald

Overview: NNL is interested in exploring TSL for solid moderators and quantum oscillators. Ab initio molecular dynamics were used to increase accuracy. New contributions to ENDF/B-VIII.1 primarily include metal hydrides.

YH_x: quantum oscillator physical phenomena have been validated against new measurements from RPI with Bragg Edges.

ZrH_x: need to incorporate both phases of Zr that can be created within the moderated, disordered alloy effect will be explored in future effects on ZrH_x

ZrC: phonon dispersion relations were consistent with inelastic neutron spectroscopy.

New thermal scattering processing methods include adaptive incident energy grids in NDEX to improve numerical fidelity of metal hydride cross sections. Several evaluations have been submitted for ENDF8.1. Additionally, some sub-thermal measurements have also been completed.

Discussion Items:

- **ACTION**:
  - ENDF/B-VIII.0 ZrH TSLs neglects crystal structure so the new submission will include coherent elastic scattering for Zr.
- **QUESTION**:
  - Which materials have already been submitted for ENDF/B-VIII.1?
    - *Response:* ZrH, Be_2C, Enriched ^{7}LiH and ^{7}LiD.
  - (Dan Roubtsov) For users, it would be useful to provide inputs for reproducibility (user can create their own NJOY files).
    - It is difficult for the NJOY developing community – do not need specialized grid for material.
    - (Andrej Trkov) Adaptive energy grids in NJOY may be a solution for mesh grid issue.
      - Let user set grid then build an adaptative mesh after. NDEX and FLASSH already have capability.
  - (Skip Kahler) NJOY/THERMR's fixed output energy grid was developed decades ago for water is a known weak spot for today's more complex TSLs and associated cross sections. A modification in THERMR to allow users to specify an output energy grid has been developed offline. A more sophisticated option to create an output energy grid on the fly (RECONR linearization) has not yet been developed but is under consideration. Also, the k_{calc} impact for smooth cross-sections like H-in-H_2O or H-in-CH_2 is much less.
    - (Trkov) A code verification project was conducted at the IAEA where the need for an adaptive energy grid was pointed out. Some of the participating codes (ACEMAKER, GRUCON) already have this capability.
- **RESOLVED**:
  - New TSL evaluations and re-evaluations for submission to ENDF/B-VIII.1 for solid moderator systems and several quantum oscillators (*Re-evaluation from ENDF/B-VIII.0, **Evaluated using LEAPR)
    - Yttrium Hydride (YH_2)*
    - Zirconium Hydride (ZrH_x and ZrH_2)*
    - Enriched Lithium Hydride/Deuteride (^{7}LiH, ^{7}LiD)
    - Beryllium Hydride (BeH2)
    - Beryllium Carbide (Be_2C)
    - Zirconium Carbide (ZrC)

        - Uranium Hydride (H-UH_3)**
    - Sub-thermal transmission measurements for Be, YH_2, ZrC, and heavy paraffinic oils have been performed at RPI.
- **DISCUSSION**:
    - Under consideration: Sub-thermal transmission measurements for ZrH, BeH_2 revision for coherent elastic scattering.

Proposed methodology for evaluating and validating TSLs

Speaker: Chris Chapman (Oak Ridge National Laboratory)

Overview: The proposed methodology is a wholistic approach to validate the TSL of entire libraries, and the case in point will be polystyrene. The phonon density of states (PDOS) was chosen to vary because it affects all forms of thermal neutron scattering. Validation of TSL cross sections have included differential cross section measurements at ORNL and RPI and PNDA experiments at LLNL. ORNL work has demonstrated with an evaluation of polystyrene to calculate some phonon properties using VASP, Phonopy, and OClimax. Photon density of states (PDOS) were optimized using NCrystal, which affects all forms of thermal neutron scattering. RPI transmission data were used to evaluate so cannot also be used to validate. Validation is being done through other double differential scattering cross sections that have been integrated over energy and angle to provide a useable and visually digestible form of data. Attempts to independently validate polystyrene evaluation using ICSBEP benchmark experiments (MCT-012 & some other Pu benchmark) were unsuccessful since delta k_{eff} due to evaluations was less than benchmark uncertainties.

Discussion Items:

- **ACTION**:
    - Experiments with multiple samples and sample sizes, some for validation and others for evaluation would be ideal.
    - Polystyrene PNDA experiment.
    - Polystyrene TEX experiment.
- **QUESTION**:
    - (Hawari) Handle uncertainty in Sequoia, specifically detectors, graphite measurements did not have better resolution than 20 meV (this depends on choice of incident energy).
        - *Response*: Thought they were fine - don't see issues.
    - (Wormald) Did you determine if the optimization process is artificial or based on physical understanding?
        - (Kemal) before we only used total cross section to do matching, an upgrade is required to combine both. All effects are constrained by both differential and total cross sections. The agreement to the differential scattering is good.
        - (Hawari) During post physical fitting, do you re-examine data?
            - (Kemal) No, we don't look at things like heat capacity since we are constrained from total and differential.
                - (Hawari+Zerkle) It is good to check these things.
    - Before fitting the RPI Polystyrene cross section, why did the ORNL evaluation overpredict, is it truly due to the PDOS?

    - *Response:* Maybe due to other compensating phonon effects.
- **DISCUSSION**:
    - (Zerkle) PCM-002 benchmarks are not the highest quality benchmarks.
    - (Zerkle) Tex experiment for Polystyrene is worth investigating, PNDA experiments are also very useful.

Status of ORNL TSL evaluations

Speaker: Kemal Ramic (Oak Ridge National Lab)

Overview: Continuation of Chris Chapman's talk. Accurate phonon spectra are required for an accurate TSL evaluation for any material/isotope. Preliminary investigation of Teflon structure (orthorhombic polymer) created more confusion due to the higher degree of constraints required. Molecular dynamics and AIMD calculations were both performed to validate the crystalline structure. No impact was observed on fast spectra benchmarks. Since new measurements are available from RPI, PE re-evaluation is important. Historical and new (RPI) measurements of polyethylene total cross section and ORNL evaluation are in good agreement. In Lucite vision measurements, ORNL does better than ENDF/B-VIII.0 for prediction but there is still a large disagreement between ORNL and data. Lucite RPI transmission data were used in Lucite evaluation PMMA as well as PNDA. New TSL library for Teflon was created and submitted to NNDC for the inclusion in ENDF8.1.

Discussion Items:

- **ACTION**:
    - Potential new measurements of Teflon (RPI) and re-evaluation of Fluorine.
    - Determine why ENDF8 and ORNL PE area under the curves in S(q,ω) as a function of energy are so different
- **QUESTION**:
    - (Zerkle) Is this an energy region that impacts experimental work?
        - (Kemal) Goes down to 25 meV.
        - PMT-004-001 is the least thermal benchmark, best agreement to ORNL evaluation.
    - (Jonathan Wormald) ENDF/B-VIII.0 vs. Revised. Why is ENDF/B-VIII.0 underpredicting S(q, ω).
        - Normalized to 1 via full area integral
            - Is this incorrect?
            - No, the full areas under the curves need to be understood
        - (Wormald) Plotted ENDF doesn't appear to have this done, normalization looks like an issue. Will need to understand why they aren't the same area to explore resolving issues.
- **RESOLVED**:
    - Teflon, poly, Lucite evaluations submitted to NNDC

TSL Nuclear Fuel Evaluations and Capabilities at NC State University

Speaker: Nina Fleming (North Carolina State University)

Overview: The objective is to provide thermal scattering law (TSL) and cross section data to support advanced reactor modeling and criticality safety. Validation is required on each step of the evaluation work presented. Phonon dispersion calculation and experimental data were compared, followed by DOS of UC. Uranium Dioxide DOS effects resulted in differences in total cross section. In material modeling (DFT and FLASSH), large valence electrons present means that a large 2x2x2 supercell (64 atoms) is required. Uranium-metal is highly temperature dependent using molecular dynamics to capture the phonon effects. FLASSH is the modern thermal scattering evaluation code which improves the physics of TSLs. It has a convenient user interface and includes advanced physics. In TSL evaluations, it is necessary to expand available U TSLs beyond UO_2 and UN. Enrichment evaluations are specifically designed to capture what we would see in a benchmark experiment by keeping the density of the states the same for each evaluation. Density of states were determined to be independent of ^{235}U enrichment. The mass and free atom cross section are changed. For each evaluation, there is benchmarking against total cross section and natural cross section data. Uranium nitride has strong coherent and incoherent scattering effects, the total coherent elastic is stored on Uranium, and the nitrogen file contains the incoherent elastic. Benchmark applications are used to see impact of TSLs. First, HEU-COMP-THERM-002 (uranium carbide, light water, polyethylene) is highly sensitive to TSLs and lowers k_{eff} by 487 pcm.

Discussion Items:

- **ACTION**:
  - Investigate if it is possible to let a user make any enrichment UO2 that they want.
- **QUESTION**:
  - (Trkov) Uranium metal crystals are known to be anisotropic. Crystal prevailing orientation depends on the manufacturing process, so I suppose it's neutronic properties can also be anisotropic. How can you deal with this?
    - *Response:* highly temperature dependent shows up in manufacturing processes – typical average value – assumes room temperature – this is how we represent experimental data
  - (Yaron) What is the ^{238}U difference in the first resonance?
    - The difference is shown at 23 K to exaggerate this is due to the impact of the structure.
  - (Yaron) Is it possible to do U5 in UO2 and U8 in UO2 separately and have a user make any enrichment that they want?
    - *Response:* Yes, it is possible.
  - (Doro) How do we tell the user which TSL to use for the different enrichment? SCALE code has different names and IDs (does things differently than MCNP)
    - *Response:* will be able to call it the same way. The evaluator needs to know the enrichment of fuel so there is a different ID (this could be complicated).
  - (Dan Rou) Cutoff for U-metal: 2-3 eV needs to match on linear scale. What about temperature cutoffs for new reactor failure temps?
    - (Colby) Everything but U-metal was taken to 2000 K, at 900 K the U-metal phase shift begins and model for TSL no longer applies.
  - (Jonathan Wormald) Have you investigated why the TSL is having such a large impact on the benchmark calculation?
    - *Response*: Investigation is still underway as far as why this is sensitive.
- **RESOLVED**:
  - New and updated uranium fuel evaluations have been submitted to the ENDF/B libraries. These include vital fuel materials U-metal, UC, UN, and UO_2.
- **DISCUSSION**:

- (Zerkle) Conscious of permutations for TSLs.

Implementation of TSL Evaluations Beyond the Incoherent Approximation

Speaker: Briana Laramee (North Carolina State University)

Overview: The goal of the work is to produce TSL libraries that contain high fidelity physics including coherent inelastic effects, which are usually ignored. Graphite and Beryllium are the important materials under consideration due to the structure. The LEIP evaluation process uses VASP, PHONON and FLASSH. Typical TSL Approximations are the incoherent approximation (S_d = 0) which assumes the distinct component is negligible, the Cubic Approximation which assumes isotropic forces (non-directional) and impacts inelastic and elastic scattering, the Atom Site Approximation which assumes all atoms are the same and the Harmonic & Gaussian Approximations which allows for use of the phonon expansion and simplifies correlation functions. Removing the Cubic Approximation impacts the TSL at higher alpha and energy regions but does not impact energy region below Bragg cutoff. Results are applied to crystalline graphite and beryllium TSL evaluations which show major improvements.

Discussion Items:

- **QUESTION**:
  - (Chapman) Convolution of phonon spectra accounts for multiple phonon scattering but the approximation shown in the talk goes to 1 Phonon?
    - *Response:* More phonon orders contribute to the TSL, first phonon order is the most important in the SD expansion. There are limited returns as you increase the total number of terms.
  - (Daskalakis) Beryllium does not extend as high as graphite does this indicate that grain size comes into calculations?
    - *Response:* Materials are fully crystalline. There are impacts in coherent elastic... extension of Bragg peaks and phonon dispersion have not been tested yet and could have an impact. Other physics can be considered in this evaluation.
  - (Wormald) Beyond experimental testing, any physics-based validation tests?
    - *Response:* Yes.
- **RESOLVED**:
  - New and updated uranium fuel evaluations have been submitted to the ENDF/B libraries. These include vital fuel materials U-metal, UC, UN, and UO_2.
  - Full MF7 submitted to NNDC for Be-met and graphite (porosity unspecified)

Covariance Committee

Chair: Denise Neudecker (LANL)
Date: Wednesday, November 2, 2022

5-10 year priorities identified for nuclear data uncertainties and covariances

Speaker: Denise Neudecker (Los Alamos National Laboratory)

Overview: The session will discuss ENDF/B-VIII.1 covariances, problems in MF=34, and a few new developments. This talk presents a list of high priorities to be addressed in the next 5-10 years on the topic of nuclear data covariances and uncertainty quantification. It came out of a virtual, invitation-only meeting on this topic that took place Oct. 11-13, 2022 (Nuclear Data Uncertainty Quantification Working Meeting). It is a NDWG meeting asked for by DOE Office of Science. The goal was to draft a whitepaper to list these priorities. Drafted white paper should provide actionable (i.e., high-level plan provided) and feasible (i.e., approximate funding level suggested) needs. A group of 30 experts across nuclear data producers and users (astrophysics, safeguards, nuclear energy, NRC, neutron dosimetry, isotope production, nuclear medicine, space needs, etc.) took part to develop these needs:

Prioritized high-level needs:

1) Purely model-based medium-fidelity covariances for all isotopes across the chart of nuclides for: (First) Neutron induced cross sections up to 60 MeV, (Second) Angular distributions, and (Third) charged particles for 250 MeV.
2) Quality assurance of covariances via standardized V&V and proper documentation.
3) Towards a more complete and easier accessible EXFOR and expert judgement database.
4) Expand training for users on nuclear-data covariances.
5) Open-source adjustment tools for general user community.

Some secondary priorities identified pertain to sensitivities for additional integral responses, covariance for TSL/FPY/stopping power/decay constants, etc., sampling tools, re-visit important nuclear-data validation experiments.

Discussion Items:

- **ACTION**:
  - Highest priority needs (cross-cutting across many subject areas):
  - [Long-term] Model-based medium-fidelity covariances across the chart of nuclide for neutron/charged particle induced reactions and angular distributions
  - [Start for VIII.1] V&V and proper documentation of covariance in evaluations
  - [Long-term] Ensure EXFOR will support growing covariance needs
  - [Medium-term] Teach user community more about covariances and how to user them
  - [Medium-term] Open-source internal adjustment tools to the community
  - Priority needs for sub-set of users:
  - [Long-term] Covariances for evaluations in sub libraries which do not currently include them
  - [Medium-term] Open-source tools for sensitivity determination to specific parameters
    - [Long-term] sampling tools
    - [Medium-term] re-visit important nuclear-data validation experiments.

- **QUESTION**:
  - (Lee Bernstein) Do we start with just input uncertainties and then forward propagate these uncertainties?

    - Answer: yes, let's start getting them, and then we worry about forward-propagating.
  - (Roberto) Even medium fidelity uncertainties are very difficult to obtain – users typically need uncertainties and covariances to agree with mean values of experimental data.
    - Answer: this is planned to be model-based providing mean values and covariances.
- **RESOLVED**:
  - NDUQM meeting took place Oct. 11-13th, white paper to be drafted on prioritized nuclear data covariance and uncertainty quantification needs that impact users.

Covariance testing and missing covariances

Speaker: Denise Neudecker (Los Alamos National Laboratory)

Overview: It is necessary to check mathematical constraints for covariance (eigenvalues >=0, symmetry, correlations 1 in diagonal, off-diagonal between 1 and -1, constraints on PFNS, sum-rules, MF=34, etc.). Counter-check if evaluated uncertainties are realistic in size (Don Smith expert judgment, standard, templates, and Physical Uncertainty Boundary test.). These counter-checks are not hard bounds but should rather give you some warning signs if something is unrealistically small or large. Processing checks will be done by Doro with reference to Don Smith for lower limits on what's valid to incorporate into MF33, 34, etc (nothing lower than 1% besides very specific range in PFNS). There are missing covariances for entire isotopes in VIII.0 (Table is shown below). These isotopes were identified by satisfying that they non-negligibly appear in our typical validation experiments (k_{eff}, β_{eff}, Rossi-alpha, spectra, LLNL pulsed spheres, subcrits) AND that no covariances are available at all for the isotope. In bold are those that cannot be processed but are available.

Discussion Items:

- **ACTION**:
  - [For all evaluators providing evaluated data for VIII.1] Please, provide covariances by Jan 2023 for ENDF/B-VIII.I
  - Complete the simple mathematical checks on the covariances before submitting them.
  - [Long-term] Add covariance for all isotopes in table above
- **QUESTION**:
  - (Andrew Holcomb) I added/augmented these checks into the latest AMPX so ORNL should be able to process and report the defective ones pretty easily
  - (Klaus Guber) So, you are essentially taking fully-correlated systematic experimental uncertainties as the bounding value for your evaluated uncertainties? What about statistical ones?
    - Answer: Yes, that is the general idea. The idea behind is that experimental data are bounding our best understanding of nuclear data and their uncertainties, where available, should drive evaluated uncertainties. Evaluated uncertainties significantly below should trigger questions.
  - (Klaus Guber) Ok.
  - (Roberto) For nuclei without experimental data, you have extensive uncertainty in TENDL. Whatever is done we probably should compare to their assessment. Experimental uncertainty is driven by systematics – are covariances too large?
  - Discuss during the break
- **RESOLVED**:

- (Nathan Gibson) Issues in NJOY have be fixed that made it previously impossible to process ^{54}Fe covariances with NJOY.

Generation of synthetic experimental data in the resonance region in support of reliable and reproducible cross section uncertainty evaluation

Speaker: Noah Walton (University of Tennessee)

Overview: Developing the ability to identify and determine resonance parameters using ML/AI. Goal is to develop data synthesis (create fake data) in order to gain more appropriate evaluated uncertainties than what is currently determined using R-matrix analysis. Sample from statistical distributions of resonance parameters to generate a pseudo-random cross section which can then be inverted to counts. Statistical distribution perturbations are then used to introduce *experimental noise* (fluctuations) to the counts. A final inverse data reduction is used to produce data that can be considered raw data from TOF measurements. Generated pseudo-data can then be used to train additional models for R-matrix analysis, data reduction processing, etc.

Discussion Items:

- **QUESTION**:
  - (Nick Thompson) Do you add in a resolution function into your simulated data?
    - *Response*: Yes
  - (Yaron Danon) We've done this before with covariance calculations... what is the next step using AI?
    - *Response*: This will be address in the Atari project – second part of thesis work
  - (Georg Schnabel) How do you plan to release the synthetic experimental data?
    - *Response*: GitHub. Data generation is very experiment specific, but the codes will be open source for users (eventually).

^{181}Ta covariances and problem of low evaluated uncertainties

Speaker: Mike Herman (LANL)

Overview: Kalman filter (LANL) brings together **curated experimental data** and model parameters.

The total cross section in ^{181}Ta is reproduced extremely well but uncertainties are unrealistically small. Unspecified sources of uncertainty (USU) have been added. Maximized uncertainties arises from 40% correlation of cross sections, but decrease with increasing correlation. This is counter-intuitive. Uncertainties from well constrained optical model parameters have little effect. If there are gaps in energy regarding experimental data, then the uncertainties will grow significantly. The number of experimental points drives posterior uncertainties down. In conclusion, the number of experimental data points drives uncertainties too small, model flexibility is critical and curating experimental data is important (removing outliers, reducing their number/thinning). It is possible to deal with single reactions at a time but then the cross-section correlations are lost.

Discussion Items:

- **QUESTION**:
  - (Georg Schnabel) Isn't the scaling only happening if using uncorrelated experimental data? As soon as normalization uncertainties on experimental datasets are added or a model

defect covariance matrix introduced, the scaling by number of datapoints should disappear, both in Kalman and generalized least squares (GLS).
    - *Response:* The case of increasing correlations (transforming statistical uncertainty to systematic uncertainty) is of course different from adding a normalization uncertainty, so my previous statement does probably not apply to your studies.
- (Jesse Brown) I've put in uncertainties up to 100 keV for ^{181}Ta, were these considered? *Response:* yes, they are in the file – the uncertainties are overwritten by those written by Jesse Brown.
- (Allan Carlson) We see here 1/sqrt(n) behavior of experimental data because you do not take into account covariances for your experimental uncertainties. Add them in. When the correlations are roughly 40%, the systematic uncertainties go up and then down
- (Roberto) (?) Experimental data constrains the shape, which the optical model cannot do .
- (Trkov) If you are making uncertainty of experimental data 100% correlated, that means you have no stability in adjusting the shape, which means anything can go up and down, so the final uncertainty will be low – this doesn't seem correct.
    - *Response*: It might be wrong but it is being tested.

FPY covariances

Speaker: Amy Lovell (Los Alamos National Laboratory)

Overview: Preliminary development of cumulative fission product yield covariance through combination of EXFOR data and BeoH (LANL in-house code) through Kalman filter is underway. ^{252}Cf, ^{235}U, ^{238}U, and ^{239}Pu all up to 20 MeV besides ^{238}U (still at 12 MeV due to continuing work on 3rd chance fission). Cumulative FPYs are largely uncorrelated due to local mass conservation. BeoH has been preliminarily demonstrated to reduce uncertainty on FPY of ^{252}Cf(sf). Correlations to ^{239}Pu and ^{235}U FPY as a function of incident neutron energy have been produced. Lower uncertainties are seen in most of the FPY calculated by BeoH relative to ENDF/B-VIII.0. Data have been shared with BNL to study impact of considering correlations for these data.

Discussion Items:

- **ACTION**:
    - Efforts are needed to collaborate with Europe and comparisons are needed to use their results.
- **QUESTION**:
    - (Chadwick) There has been work on this, mainly in Europe can you comment? Have to look deeper first in order to understand the covariance models employed and what's going on.
    - (Kawano) Meeting in December with international collaboration
    - (Denise) The model brings uncertainties down, is this well-justified or a result of the stiffness of model?
        - *Response:* It's something we need to look into more. Also, in some cases, experimental uncertainties are below the calculated uncertainties and below ENDF. We need to understand those.
- **RESOLVED**:
    - Preliminary covariances calculated for ^{252}Cf(sf), ^{235}U, ^{238}U, and ^{239}Pu (all n,f).
    - Submitting FPY covariances for ENDF/B-VIII.I. So, evaluations will include these covariances for the first time

- **DISCUSSION**:
  - The final covariance format for ENDF/B-VIII.I is still actively being discussed.

Impact of FPY correlations
Speaker: Alejandro Sonzogni (NNDC - BNL), Andrea Mattera (BNL)

Overview: Talk was not presented.

RRR actinide covariances
Speaker: Marco Pigni (ORNL)

Overview: No results yet; however, the strategy for ^{235}U and ^{239}Pu will be discussed. Evaluated uncertainties are reflection of the accuracy that can be reached on measured nuclear data. Consistency is needed on how covariances are reported. Many experimental effects are accounted for when fitting experimental data in SAMMY. Boosting the uncertainties on resonance parameters may not be the best approach. Tendency to match the experimental uncertainty can lead to an increase in uncertainty from theoretical calculations. Marco argued that the model uncertainties should be the main driver. Need to be able to separate the experimental uncertainties from experimental data and convolute them with the resonance parameters (theory that isn't just artificially enhanced to match experimental uncertainties.) This is to address the resolution affects from fitting regime, very important for sharp and/or self-shielded resonance.

Discussion Items:
- **DISCUSSION**:
  - (Danon) comment: the SAMMY fit uncertainty comes too low compared to experiment. Because we do not include all correlations, it is difficult to back out experimental correlations.
    - In theory there is not a lot of flexibility to change energy of resonances, for example. Can only be accounted for via experimental effects.
    - Response: pure R-matrix theory is used for fitting resonances. Resolution is an experimental effect.
  - (Danon) uncertainty has to reflect differences in experiment and theoretical results such that the model is constrained
  - (Denise) agrees with Danon. But what if you miss a resonance, or are not quite sure where the resonance should be? Do you consider that uncertainties?
  - (Marco) We have a stiff model and I take choices.
    - Without experimental data, model cannot predict anything.

^{235}U and ^{239}Pu PFNS and nu-bar covariances
Speaker: Denise Neudecker (Los Alamos National Laboratory)

Overview: The ^{239}Pu evaluated uncertainties obtained with the Los Alamos models are unrealistically small. So, they were increased with a normalization factor of 2.1. ^{239}Pu nu-bar uncertainties are lower than ENDF/B-VIII.0 due to Marini high-precision experimental data (2022, not included in ENDF/B-VIII.0) & CGMF. ^{235}U(n,f) PFNS evaluated uncertainties with Los Alamos model are unrealistically small, so they

were multiplied with factor 4.9. The new PFNS uncertainties are lower than those in ENDF/B-VIII.0 given that Chi-Nu high-precision experimental data are included. Evaluated ^{235}U nu-bar uncertainties enclose majority of experiments. New evaluated ^{235}U nu-bar uncertainties are distinctly larger than ENDF/B-VIII.0 due to new standard uncertainties. The standard ^{252}Cf nu-bar uncertainties of 2011 were 0.15% and increased to 0.42% for 2018. This resulted in an increased ^{235}U nu-bar uncertainty from 0.3% to 0.5%. Users please be aware that there is a large change.

Discussion Items:

- **ACTION**: Increased ^{235}U nu-bar uncertainties should be communicated to users sooner rather than later.
- **QUESTION**:
    - (Nathan) Should there be cross correlations included for PFNS across multiple incident energies?
        - Response: seems like this is a good time to revisit for GNDS if there is time and desire to improve.
    - Current work around with multiple chance fission works well for energy correlations for PFNS and keeps the size more reasonable. Full correlations would result in a 16,000x16,000 matrix with not much added benefit given the energy range pertinent for applications.
    - Why do we keep changing the uncertainties in different directions? Users confused.
        - ^{239}Pu nu-bar uncertainties were revised already for ENDF/B-VIII.0 using the new ^{252}Cf(sf) nu-bar uncertainties from the 2018 standards, but nothing was done for ^{235}U nu-bar. This was a mistake in ENDF/B-VIII.0 that is now being corrected.
        - We keep reversing between Pu/U uncertainties, with one uncertainty coming down and another coming up with each release.
    - (Georg Schnabel) If PFNS covariances include the normalization constraints, will this pose a problem to codes further down the pipeline due the matrix having not full rank anymore?
    - (Talou) not sure I understand your question about PFNS covariance normalization constraint? If we consider PFNS to be a normalized probability distribution, then any perturbed PFNS sampled from the covariance should also be normalized. Is this what you are referring to?
    - (Schnabel) Yes. The constraint is required from a definition point of view. However, some codes may use a Cholesky decomposition or similar for sampling from a covariance matrix, which requires the matrix to be positive definite. The normalization constraint would make the covariance matrix positive-semidefinite as it reduces its rank by one. Is there any understanding whether codes used at present for Monte Carlo uncertainty propagation can deal with such a covariance matrix?
    - (Talou) interesting point. While the original Cholesky decomposition requires a positive-definite matrix, I believe there are several techniques/tools that have been developed to adapt the method to a semi positive-definite matrix. From what I know with Monte Carlo uncertainty propagation is the use of Principal Component Analysis instead. I don't know if Cholesky might be better in some cases, e.g., memory use?
    - (Schnabel) Yes that's true. Extensions of Cholesky and SVD don't have the problem. It was more a pragmatic question about codes in use.
    - (Dan Roubtsov) for ^{239}Pu (n,g), ^{239}Pu (n,f), etc., Do uncertainties / covariance of the negative energy resonance parameters have sense? (Bound level energies) Say, if we do

MC sampling of, say, ^{239}Pu resonance parameters, shall we include the sampling of "negative" resonances E & widths? (Do we have them available for ^{239}Pu?)
        - Unanswered.
    - (Andrej Trkov) Is your re-normalization of PFNS uncertainties arbitrary or is it based on something physical?
        - Los Alamos model parameters are too restrictive. They give evaluated uncertainties that are distinctly to small compared to experimental data. An evaluation was undertaken with experimental data only to give an estimate of the minimum evaluated uncertainties that are reasonable. Evaluated uncertainties with the model are re-scaled to that extent.
    - (Talou) It's a good point. Just remember that evaluated uncertainties are no different than evaluated mean values. They change with every new version, if we have new information. If we want to be more conservative, especially from the NRC perspective for instance, we should take into account the estimated uncertainties on the evaluated uncertainties. This could be done by estimating ranges of uncertainties and correlations in the experimental data, and to some extent in the model variations themselves. Another challenge for sure.

Adjusting nuclear data to multiple responses beyond k_{eff}
Speaker: Jesson Hutchinson (LANL)

Overview: EUCLID will execute validation experiments optimized to resolve compensating errors between ^{239}Pu PFNS, nu-bar, fission, elastic, capture, and inelastic cross section. We will adjust nuclear data to new and existing experiments to assess impact of new measurement. Additionally, EUCLID provides sensitivities for many measurement responses with respect to nuclear data. PMF-001 (Jezebel) k_{eff} adjustment leads to small changes in nuclear data mean values but very large changes in the covariances as nuclear-data mean values are tweaked to it, but covariances remained unchanged. PMF001 ^{239}Pu /^{235}U and ^{238}U/^{235}U reaction range adjustment has a large impact on Jezebel k_{eff} (drop of 715 pcm). Adjustment with PMF001 neutron leakage spectra for fission cross section is somewhat similar to jezebel k_{eff} experiment-with k_{eff} change of 150 pcm. Additional adjustments include PMF001 reactivity coefficient (Pu L1 only), PMF001 reactivity coefficient (Pu all locations), PMF001 reaction rate ratios, reactivity coefficients (all locations, and neutron leakage spectra).

Discussion Items:

- **ACTION**:
    - Two new experiment configurations (high mass, slab like and low mass similar to Jezebel) will be constructed at NCERC.
- **QUESTION**:
    - How do we design an experiment to optimally reduce unconstrained physics spaces? What new experimental data would lead to the most constrained nuclear data?
    - Currently designing an experiment at NCERC focused on ^{239}Pu reactions: PFNS, nu-bar, (n,el), (n,inl), (n,g), and (n,f).
    - Why was the determinant optimized? Why not use other optimization schemes like A, B, C – optimality?
        - Response: question for ML experts on our team – many discussions and other types were considered

- Denise – D optimization allows us to incorporate covariances into the nuclear data uncertainty optimization

- **DISCUSSION**:
  - Reactivity coefficients may be of interest for future validation efforts.

LANL Cross Section Covariances

Speaker: Matthew Mumpower (Los Alamos National Laboratory)

Overview: We are in the process of updating the ^{239}Pu cross sections in the fast energy range (complementing the work of IAEA / INDEN / ORNL / LLNL). Covariances were constructed with NEXUS KALMAN code by combining model variation with experimental uncertainties. Bayesian inference was used to estimate covariances. Soukhovitskii (2005) optical model [deformation ~0.21] was used for ^{239}Pu(n,tot). The uncertainties were generated from a variation of 7 optical model parameters and 25+ experimental datasets. The results show a generally positive correlation as a function of energy. CoH statistical Hauser Feshbach with M1 of Mumpower et al. PRC 96 024612 (2017) was used for ^{239}Pu(n,tot). LANL relative uncertainty for both reactions are consistently higher than ENDF/B-VIII.0. CoH with new collective enhancement of Mumpower et al. submitted PRC (2022) for ^{239}Pu(n,2n). CoH statistical model was also used for ^{239}Pu(n,inl).

Discussion Items:

- **ACTION**:
  - Investigate why LANL produced uncertainty on total and capture cross sections of ^{239}Pu larger than in ENDF/B-VIII.0.
- **QUESTION**:
  - (Potel) Does the variation of the model parameters introduce cross-correlation between different cross sections?
- **DISCUSSION**:
  - (Denise) the uncertainties in ENDF/B-VIII.0 started one bin too late for the (n,inl) and (n,2n) cross sections.
  - This has been corrected.

Problems in MF=34 covariances

Speaker: Kent Parsons (Los Alamos National Laboratory)

Overview: There exists limited availability of mubar (messed up beyond all recognition) covariance data (so far, ~100 isotopes). The only (major) isotopes are ^{16}O, ^{235}U, ^{238}U, ^{239}Pu and among those missing are H, D, Be, Li, B, C, N, ^{27}Al, ^{56}Fe, and ^{240}Pu. Physical limits on absolute mubar covariances: their absolute values must be less equal than 1.0 (future evaluations should honor this constraint). Two (ad hoc) proposed methods for limiting mubar uncertainty in random sampling are transforming to Uniform (Flat) Distribution or to truncated Normal Distribution with smaller standard deviation. In conclusion, more MF 34 data is needed and some MF 34 mubar covariances in ENDF/B VIII.0 are too large.

Discussion Items:

- **ACTION**:
  - (Denise) Limits for Angular Distributions should go in the ENDF manual.
- **QUESTION**:
  - (Denise) You mentioned something about ^{235}U, ^{238}U, can you share?

- There was an NJOY fix the ^{235}U and ^{238}U came from Roberto. The data was originally not able to be read or manipulated with NJOY. Resolved.

NJOY and processing MF=34
Speaker: Wim Haeck (LANL)

Overview: MF34 has sub-subsections which were largely ignored previously since they weren't used. However, eventually ^{235}U did use the sub-subsections and this broke NJOY. The crash issue has been resolved but needs an updated output format. A temporary work around can be achieved by placing the desired sub-subsection in the first entry of the file. NJOY will read and execute the first sub-subsection listed.

Discussion Items:

- **QUESTION:**
  - (Denise) Is this an easy fix?
  - Is there enough space to add Legendre polynomials?
  - Don't think it will be a formatting issue
  - Another option: specify which energy range you want
  - We don't like that because as users because we have to repeat operations and then the output is in a different section (does not sound effective)
- **RESOLVED**:
  - Users were pleased – agreed that an update in GNDS is needed

Problems in formulating MF=34
Speaker: Roberto Capote (IAEA NDS) presented by Andre Trkov

Overview: ^{235}U reaction-wise uncertainty of k_{eff} in Godiva has a main contributor of (n,n') in JENDL-5 but in ENDF8.0, the main contributor is (n,f).

Discussion Items:

- **DISCUSSION**:
  - (Denise) we are actively learning about how to do this process correctly.

INDEN Pu-239 (n,g) and (n,2n) covariances and corrections to U-235 covariances
Speaker: Roberto Capote (IAEA NDS)

Overview: Uncertainty quantification methodology includes a generalized least squares model of selected experimental data and reaction modeling results. Evaluated uncertainties were reduced. Any covariance relies on the nuclear data input. GANDR fit reduces and enhances capture cross section in different energy regions. $\chi 2$ was evaluated using ^{239}Pu capture data. Of the INDEN and ENDF evaluations, INDEN generally performs better. Different evaluations agree within uncertainties for ^{239}Pu(n,2n) cross section. Uncertainty reduction was achieved by making use of experimental data uncertainties and covariances by latest reference values and uncertainties.

Discussion Items:

- **ACTION**:
  - Nu-bar for ^{239}Pu to be discussed below 300 keV as model leads to higher values but experimental data are also uncertain and scattered. New measurement will come from CEA to shed some light on this. Revisit for ENDF/B-IX.0.
- **QUESTION**:
  - (Patrick) Your chi-square values look very small. Are you worried about over-fitting?
    - *Response:* No [rapporteurs could not understand the reasoning]
  - (Denise) Do you account for energy uncertainty for (n,gamma) measurements?
    - *Response:* It is unclear at this point if GANDR takes this into account. (Denise): This needs to be investigated for ENDF/B-IX.0 along with a full analysis of experimental data in the field.

Measurements Committee

Chair: Yaron Danon (RPI)
Date: Wednesday, November 2, 2022

LANL results on $^{16}O(n,\alpha)$

Speaker: Hye Young Lee (LANL)

Overview: JEFF3.1 and JENDL4.0 are very similar to ENDF/B-VII.1 for the $^{16}O(n,\alpha)$ cross section. With better understanding of systematic uncertainties associated with (n,z) reaction measurements at LANSCE through multiple reaction studies and validations with MCNP/GEANT simulations, we provided differential cross sections on the $^{16}O(n,\alpha)$ reaction with experimental resolution functions. To reduce uncertainties for LANSCE measurements, we investigated direct measurements of reaction cross sections, ratio method with reference cross sections and Forward Propagation Analysis by validating available libraries in MCNP6. Future measurements at LANSCE include a diamond mosaic array for better neutron energy resolution and ~90-degree detection. Additionally, a TPC detector for better neutron energy/angular resolution can also be used. This work suggests the need of a full evaluation including old and new data sets and differential/total cross sections, with realistic uncertainties in absolute normalizations from measurements. More effort is needed in performing consistent evaluation including high energy, break up channels.

Discussion Items:

- **ACTION**:
  - Full evaluation with old and new data sets and differential and total cross sections
- **QUESTION**:
  - (Marco) will the data be available sometime in EXFOR?
    - *Response*: The paper is being reviewed; the difficulty is the resolution.
  - (Roberto) Can you say that ENDF/B-VII.I is a better fit of (n, α_0) above 6.4 MeV, while ENDF/B-VIII.0 sum of (n, α_1+n, α_2+n, α_3+n) was properly captured in NDF/B-VIII.0?
    - *Response*: Angular distribution may be why ENDF/B-VIII looks better but for low energy this is not necessarily true

(n,z) results on Fe and Ni, including Ni-56

Speaker: Sean Kuvin (LANL)

Overview: The Low Energy (n,z) experimental station (LENZ) detects outgoing charged particles using double-sided silicon strip detectors in a compact setup close to the target sample. WNR Facility at LANSCE produces fast neutrons with a broad energy spectrum ~100s of keV to ~100s of MeV. Measurements of (n,z) reactions on ^{54}Fe, ^{56}Fe, ^{58}Ni, ^{60}Ni have been completed. The first direct measurement of neutron induced reactions on ^{56}Ni (and ^{56}Co) was also done. Pulse shape discrimination can be used to discriminate based on rise time of pulses (alpha, deuteron, proton can all be discriminated). There is general agreement between current nuclear data libraries and the Ni(n,xp) and Ni(n,nα) reactions. $^{60}Ni(n,\alpha)$ shows largest disagreement (8 – 15 MeV). Measurements have also been conducted of $^{59}Ni(n,\alpha)$ and $^{59}Ni(n,p)$ for which results are now published. ^{59}Ni is a longer-lived

radioisotope that led to some background issues in ^{56}Ni measurements. Measured ^{56}Ni(n,p) reaction for validation of nu-p reaction for nucleosynthesis.

Discussion Items:

- **ACTION**:
  - Fast and thermal measurements of ^{39}K, ^{40}K, and ^{35}Cl
- **QUESTION**:
  - (Capote) What does consistency mean? If you measure by activation, you measure the residual. If you measure directly d, p, a, then you will see (n,d) separately from (n ,n+p)

PFNS for ^{235}U and ^{238}U, and neutron scattering measurements at LANL

Speaker: Keegan Kelly (Los Alamos National Laboratory)

Overview: Experiments of the PFNS for ^{235}U were conducted at WNR at LANSCE with the Chi-Nu system. The data will be made available to guide the new PFNS evaluations. ^{238}U PFNS is still preliminary but should be completed and finalized within one month. ^{240}Pu preliminary results were shown to conclude there is enough data available to be pleased with final results. Spontaneous fission is measured with Li-glass detectors so liquid scintillators can be extended to lower energies. Since all actinides measured on consistent experimental setup, a correlation matrix describing relationship between each target and sample can be determined. CoGNAC employed an n-g approach to scattering using an iterative unfolding of neutron spectra. This improves resolution of state excitations and corrects for environmental neutron scattering events. ^{12}C(n,n'g) cross section was measured using liquid n-g, liquid g and CLYC g (but the measurements may not be completely trustworthy).

Discussion Items:

- **ACTION**:
  - Fine tune MCNP at edges of liquid scintillator data (^{238}U)
  - Determine fission fragment angular anisotropy impact (^{238}U)
  - Further analysis of ^{240}Pu results
  - Multiple scattering results will be published sometime next year.
- **QUESTION**:
  - (Talou) Do you trust the drop in the mean PFNS energy near 4 MeV?
    - *Response*: could be statistical fluctuations but I am unsure so you should not fully trust.
    - Nubar has the same issue for this energy range (2-4 MeV).
  - (Hale) We now are getting the low-energy bump coming from the 9/2+ resonance, and there are some interesting differences at higher energies.
    - *Response:* There are indeed differences, it is interesting to see how high we can push the energy for this technique.
    - (Hale) **We would like to push the R-matrix analysis above 6.5 MeV, but that requires adding at least the α+^{9}Be channel, and a lot more experiment data. We will do as much as we can with the time available for VIII.1.**
  - (Capote) Can you say something about ^{252}Cf(sf)?

        - *Response*: Cf can be used to determine efficiency of detector array. Downscattering is different for each nuclide and incident energies. Kelly *et al.,* NIMA 1010 (2021) 165552
    - (Danon) How was your response scattering unfolding function determined?
        - *Response:* it was calculated (simulated) and will be validated with measurements.
    - (Mark Paris) Was there a shift to the Geel data?
        - *Response:* No and they can go up to about 8 MeV.
- **DISCUSSION**:
    - (Denise) there will be a Cf PFNS measurement within the next 2/3 years.

Recent measurements on ^{13}C, ^{7}Li, and ^{19}F at the University of Kentucky with a digital data acquisition system

Speaker: Jeffrey Vanhoy (US Naval Academy)

Overview: There is a large 7 MV Van DeGraff generator to produce charge particles incident on a ^{3}He target to produce neutrons. HPGe detector capabilities are being expanded in the near future. New digital data acquisition systems have been developed using 500+100 MS/sec CAEN digitizers. Proper collecting of the digital data is difficult. A new digitizer system was installed to record time-dependent gamma-ray spectra and observe time dependence of background. The goal is to remeasure ^{13}C. Overall, ^{7}Li agrees but there is some discrepancy due to over-subtraction from mis-sized blank sample. ^{19}F was measured but was challenging due to 90 ns isomeric state. ^{19}F is was mentioned to be evil (see below).

Discussion Items:

- **ACTION**:
    - Re-can the ^{7}Li sample to correct for over-subtraction issue
    - Expand HPGe detector capabilities
    - Understand and correct for multiple scattering and other experimental issues
- **QUESTION**:
    - (Danon) Were there any neutron measurements of ^{19}F?
        - *Response:* There was not because of the limited neutron resolution.
    - (Capote) There is a (n,n'y) measurement on EXFOR that reports an angular distribution for first and 2nd level, show isotropic. Could you use Morgan and Dickens data to compare with your data? We proposed a much lower inelastic in our beta0 file
    - (Adam Daskalakis) Are there self-shielding issues from can?
        - *Response:* No, we tested and calculated this.

Overview of Nuclear Data Measurements at RPI

Speaker: Yaron Danon (Rensselaer Polytechnic Institute)

Overview: Capture and transmission measurements at RPI were conducted of an enriched ^{54}Fe sample. The RPI capture data agrees with previous n_TOF capture data. A new resolved resonance region evaluation will be conducted, and all data covariances will be reported. Using the RPI y-multiplicity detector array, it is now possible to collect digital data and fully collect pulse waveforms using a new digital DAQ system. Measurements are underway to validate capture gamma spectra of various isotopes and new simulation strategies are being developed with MCNP, DICEBOX, and CGM. These changes are required to accurately reproduce capture gamma spectra using simulation tools. PNDA measurements are also being done at RPI to validate TSLs. Water and polyethylene measurements have been conducted at various temperatures. There is useful data that can be collected by performing measurements at cold temperatures. WINS-2023 is being hosted at RPI.

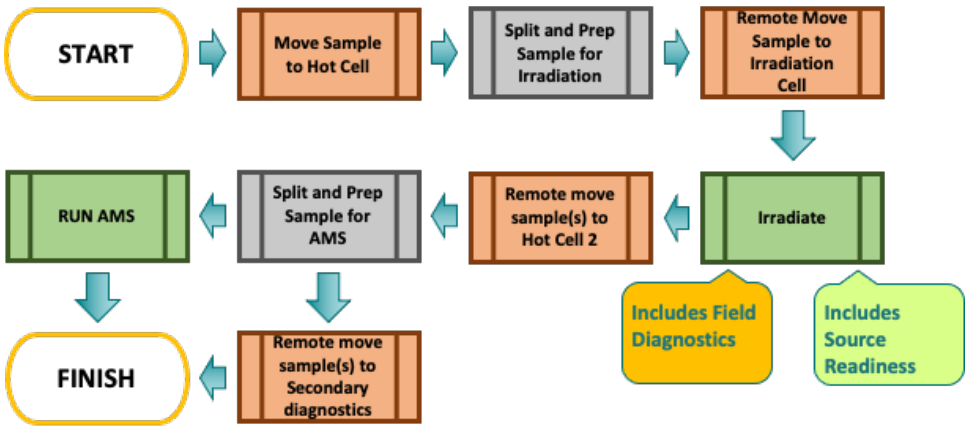
Discussion Items:

- **ACTION**:
  - Complete analysis of RPI Fe data.
  - Complete experiments to validate capture gamma ray spectra for various isotopes.
  - Complete PNDA measurements of various materials.
  - WINS Sign up: https://indico.cern.ch/event/1201892/
- **DISCUSSION**:
  - (Zerkle) Low temperature PNDA measurements are useful for criticality safety.

Nuclear Data Measurements at AWE

Speaker: Andrew Simons (AWE)

Overview: ASP is a Cockcroft-Walton accelerator generating D^{1+}, D^{2+}, and D^{3+} molecular beams that impinge titanium tritide or titanium deuteride targets generating ~14.7 or 3.0 MeV neutrons. It is primarily used for neutron hardening of electronics but has also been converted to a system which can provide neutron cross section data. Data has been collected for $^{89}Y(n, 2n)^{88}Y$ and ^{89}Y inelastic. Variable Energy Neutron Output Machine (VENOM) is a project to deliver a fast neutron capability for AWE. The project is currently in the conceptual design phase and uses two accelerators which can provide neutrons with energies 0.5 to 23 MeV with fluence over 10^{10} n/cm^2. The ultimate goal is to explore long lived radioactive isotopes, moving one to two steps away from the valley of stability.



Discussion Items:

- **QUESTION**:
  - (Danon) What is the ultimate measurement goal? And to what accuracy?
    - *Response:* 5% uncertainties on cross section measurements. High fidelity cross section measurements are done via activation measurements. The ultimate goal was simply to prove that cross section measurements are possible.
- **RESOLVED**:
  - Deuterium target was added to the machine to improve experimental capabilities before VENOM.

Sub-Thermal Transmission Experiments of Organic Materials at the RPI Gaerttner LINAC Center

Speaker: Adam Daskalakis (Naval Nuclear Laboratory)

Overview: Preliminary results are shown, blame Mike Rapp (rappm2@rpi.edu) for any issues. Enhanced thermal target cold moderator was developed by D. Fritz and used for transition measurements using a ^{6}Li glass scintillation detector. Petrolatum, Apiezon M-Grease, and DTE-24 were all measured and special care was made to prepare the experimental samples. Importance of these samples is in crit safety applications; all materials are variations on parafanitic oils. PNDA experiments should be done to validate the TSL results. There is slight improvement over the ENDF/B-VIII.0 H-C_2H_4 at low energies (below 2 meV).

Discussion Items:

- **ACTION**:
  - Fine tune experimental details and analysis
  - Results will be published and uploaded to EXFOR
- **QUESTION**:
  - (Carlson) How about sample characterization?
    - *Response:* Lots of work was put into the chemical characterization of the samples and efforts are still ongoing.

Current status of ^{90}Zr experiments

Speaker: Jesse Brown (ORNL)

Overview: The objective is to improve resonance parameter evaluations for various Zr isotopes. We are set up to run through 90,91,92,94. We will be using the ORNL ^{90}Zr transmission and capture data in addition to transmission data from Harvey/De for RRR/URR. Current capture data on EXFOR has ZrO_x in aluminum canisters, so there are lingering issues with background. Preliminary results from ^{90}Zr transmission and capture measurements show the ability to resolve discrepancies in current major international evaluations.

Discussion Items:

- **QUESTION**:

- (Ester) Have you thought about using REFIT to do the R-matrix analysis for the GELINA data?
  - *Response*: I develop SAMMY so I will be using SAMMY.
  - (Klaus) We need the correct resolution function, which we have in SAMMY. The choice of code is up to the evaluator.
- (Trkov) Why skip ^{96}Zr? It is of interest for dosimetry.
  - Response: It is a minor isotope; we would be happy to measure it if there is a strong motivation. Since this is from NCSP, it may not be available.
  - ^{96}Zr has very different resonance structure. It is interesting to measure the activation for spectrum unfolding.
  - **Continued discussion will be had about this possible measurement**

Recent Standards work

Speaker: Allan Carlson (NIST)

The Neutron Cross Section Standards

Reaction	Energy Range
H(n,n)	1 keV to 20 MeV
^{3}He(n,p)	0.0253 eV to 50 keV
^{6}Li(n,t)	0.0253 eV to 1 MeV
^{10}B(n,α)	0.0253 eV to 1 MeV
^{10}B(n,$\alpha_1\gamma$)	0.0253 eV to 1 MeV
C(n,n)	10 eV to 1.8 MeV
Au(n,γ)	0.0253 eV, 0.2 to 2.5 MeV, 30 keV MACS
^{235}U(n,f)	0.0253 eV, 7.8-11 eV, 0.15 MeV to 200 MeV
^{238}U(n,f)	2 MeV to 200 MeV

Overview: There is currently a lot of work to do on standards. H(n,n) angular distribution measurements were conducted that go up to 52 MeV with the goal to increase energies up to 350 MeV. Extensive measurements of the ^{6}Li(n,t) cross section were completed for neutron energies of 1 eV - 3 MeV. Angular distribution data were also obtained for the boron standards from 1 eV to 2.5 MeV. Carbon cross section measurements differ by 1.5% in the old and new standards, where RPI measurements are in better agreement with the old (2006) standard. U-235 and U-238 fission cross section measurements were conducted at n_TOF and extend from 10 to 66 MeV and agree with the current standard. New n_TOF measurements to 1 GeV wIll hopefully allow the standard to be extended and improved. ^{239}Pu fission cross section ratios from LANSCE (^{239}Pu/^{235}U(n,f) ratio) are above standards by about 2% and are recommended for use as ratio shape data. There was a 0.3% increase of this ratio for the INDEN cross sections.

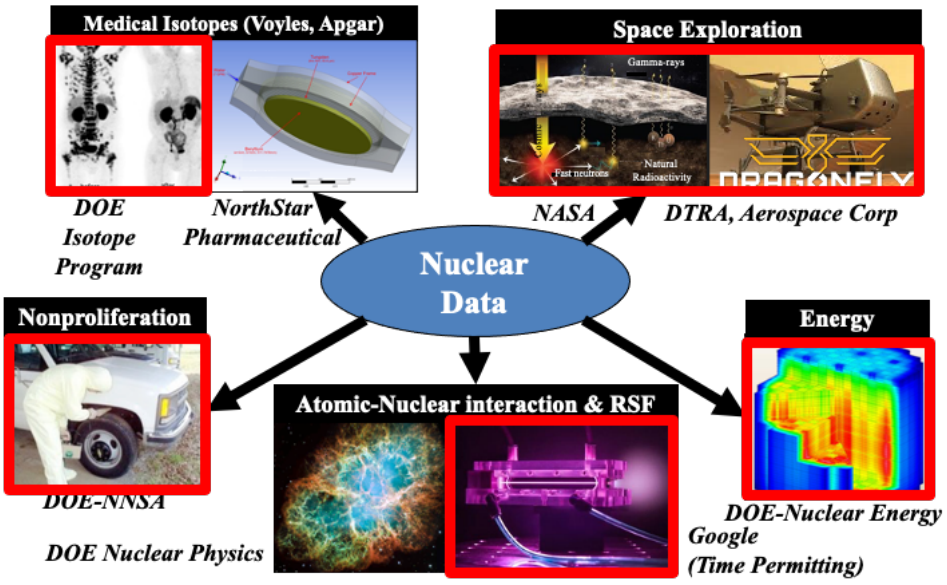
Discussion Items:

- **ACTION**:
  - Improved experimental work is necessary for all the standards.
    - Focus on **boron and lithium standards** so the upper energy bound can be increased.
    - Also, **gold capture has some of the largest uncertainties** for the standards.
  - Extend the hydrogen standard to about 150 MeV (Hale & Paris).
  - Further work on unrecognized sources of uncertainty (energy dependence of USU).
  - Consider improved evaluation techniques for the standard cross sections.
- **QUESTION**:
  - (Dave Brown) Does using SACS resolve the NIFFTE measurements?
    - *Response:* It improves NIFFTE but NIFFTE measurements still may have normalization issues.
  - (Jesse Brown) Why does one datapoint on C standard have one significantly different datapoint at ~250 keV.
    - Maybe there's a resonance ^{13}C or something? We should remeasure.
      - (Gerry Hale) That is the energy where there is a strong resonance in ^{13}C.

Measurements Program Update from Berkeley

Speaker: Lee Bernstein (LBNL/UCB)

Overview:



It is possible to determine isotope production rates at different beam energies using the stacked target method, where the decay rates of unknown targets can be examined relative to those of known targets for (p,x) cross sections. These measurements have identified optimal exciton model parameters

for p+^{93}Nb, ^{75}As, ^{139}La and ^{121,123}Sb. The Gamma Energy Neutron Energy Spectrometer for Inelastic Scattering (GENESIS) was built to measure coincident (n,xng) cross sections. ^{56}Fe GENESIS data 2+ to 0+ (847 keV) gated neutron data have been measured. ^{35}Cl(n,x) measurements were conducted using multiple experimental locations. For example, the energy differential ^{35}Cl(n,p), (n,a) and (n,n'g) cross sections and the energy integrated ^{35}Cl(n,p), (n,α) cross sections. A novel double TOF experiment setup was developed as well as GENESIS (EJ-309/HPGe) for coincident (n, xny) cross sections. The combination of HPGE and neutron detectors at 0.5m allows for high-resolution gamma-ray and neutron differential and energy-integrated cross section measurements.

Discussion Items:

- **ACTION**: Analysis is underway for 2021 and 2022 measurements.
- **DISCUSSION**: ^{96}Zr is indeed very interesting.

Status of the EXFOR project

Speaker: Boris Pritychenko (NNDC, BNL)

Overview: Historically the nuclear data compilations have been available worldwide after WWII. It was transferred from the sigma center to NNDC (where it has been for 75 years). Currently EXFOR possesses over 24,000 datasets from nuclear data experiments. The process of submission to EXFOR can be slow, but the end product is superior. The LANL library provides millions of unclassified documents. EXFOR NNDC compilation efforts are very complex and well-organized. Current and missing previous data are recovered and existing entries are revised.

Discussion Items:

- **ACTION**: 1938 measurement of (n, α) rate from LANL needs to be sent to Boris.
- **QUESTION**:
  - EXFOR is only allowed to make changes if the error in EXFOR is obvious. WPEC-SG50? Will have a library that is parallel to EXFOR entries.
- **RESOLVED**: 158 new compilations, 210 updated compilations.

EXFOR, GitHub and license issues

Speaker: Arjan Koning (IAEA)

Overview: "Open science" as defined by UNESCO is making scientific research and data open to all. To uphold open science principles, we must follow FAIR. EXFOR is run by NRDC and is surprisingly close to FAIR ideals. However, the format is old and complex. A new project from WPEC-SG50 is seeking to make data accessible and curated. The first step in the process is to compile EXFOR data from publications in 13 datacenters. Next, data is checked among NRDC. Data is stored (create, update or delete) in the system. Finally, provide interface to end users via X4, C4, C5 formats. Many people have approached the database (EXFOR) and created secondary assessable libraries to be able to strip information and use in accompanying code systems (an example is Nuclear Data Plotter https://nds.iaea.org/dataexplorer/?target_elem=Au&target_mass=197&reaction=n%2Cg). Protection

and conditions for those submitting to nuclear database, intellectual property rights, warranties, etc. Open data is data that can be freely used, re-used, and redistributed by anyone subject to the requirement to attribute and share alike.

Discussion Items:

- **QUESTION**:
  - Is CC0 or CC-BY 4.0 suitable for nuclear data and nuclear application communities?
  - EXFOR is an important example here, what about other databases? ENSDF?
  - What does CSWEG/USNDO think of all this?
    - (Dave Brown) we've been asking this question for a while now – we have released ENSDF, XUNDL without DOI's but we haven't talked about licenses
      - (Arjan Koning) Would feel better if this was under control
  - (Marco Pigni) Assuming you get a license from EXFOR and want to use a data set, should I reference EXFOR or the literature directly?
    - *Response:* It would be good if EXFOR would get more citations than it currently is, past OMP work has shown that people cite just the differential data but there is additional information that was taken from EXFOR entries and not disseminated.
  - Mike Herman – EXFOR is one case on one extreme, where people use differential authors and don't label EXFOR where ATLAS is normally referenced and differential never mentioned.
    - Agrees we need a middle ground.
  - (Nick Thompson) Is there a main EXFOR paper to cite? For example, many people cite the MCNP manual for citing MCNP. Citing the specific entry would be a good idea as well. We have the same issue with citing ICSBEP benchmarks.
    - (Devin Barry) Yes there is. **You can see an example of how to cite EXFOR here: https://www-nds.iaea.org/nrdc/about/citation-exfor.html**
  - (Boris) Discussion on public data policy that can be established where a reference can be made but the individual taking the data and sharing it does not have the right to reproduce this infinitely
  - (Amber Cole) Is the creative commons the only option?
    - (Dave Brown) That's a good question, but CC licenses capture the spirit of what we want to do
    - (Amber) Many of the other licenses were invented to cover software, unlike CC, but may offer finer detail options. https://choosealicense.com/
    - (George Schnabel) If one looks at how git fingerprints commits and objects, it's actually some kind of blockchain already. The proof of work part is missing but maybe not necessary for databases.
  - (Roberto) When writing about experimental data, you need to provide both publication and EXFOR since one is digitized and the other provides the raw information as it was presented.
  - (Mark Paris) Can a BibTex entry be autogenerated with the EXFOR entries so linking can happen on the fly?
    - It's already there but in a separate file.
    - Can the EXFOR entry number be added to the BibTex?
      - Yes, I will talk with the others.

RESOLVED: 158 new compilations, 210 updated compilations.

- **DISCUSSION**:
    - (Keith Jankowski) A recent Office of Science and Technology Policy (Whitehouse / OSTP) memo on making federally funded data public. Various agencies are working on the interpretation and implementation: https://www.whitehouse.gov/ostp/news-updates/2022/08/25/ostp-issues-guidance-to-make-federally-funded-research-freely-available-without-delay/
    - (Denise) reproducibility idea?
        - DOI persistent entry may be too much as EXFOR is continually updated and the master file is created periodically. This is very discussable.

Evaluation Committee [Fission Products and Decay]

Chair: Toshihiko Kawano (LANL)
Date: Thursday, November 3, 2022

Status of the updated FPY evaluation for 252Cf(sf), 235,238U(n,f), and 239Pu(n,f)

Speaker: Amy Lovell (Los Alamos National Laboratory)

Overview: Combinations of experimental data and model calculations through a Kalman filter optimization were presented. Covariances were calculated consistently from the Kalman filter. Bulk optimization was performed to experimental cumulative FPYs but more work is needed to ensure adequate model elasticity. Overall, there is reasonable agreement between data, ENDF/BVIII.0, and present work for mean cumulative FPY values. A piecewise approach is used to fit neutron-induced fission reactions. A process has been set up to validate select cumulative FPYs with critical assemblies. Cumulative fission product yields are systematically lower due to model (BeoH) rigidity, will be relaxing some fitting and then re-evaluating the cumulative FPY to gain better agreement with integral experiments. There is a need to make new MF38 for FPY covariance which will not be including cross correlations for outgoing neutron energies.

Discussion Items:

- **QUESTION**:
  - (Dave Brown) Don't like MF38, probably won't include all info required, will have to reinvent the wheel for GNDS anyway so let's think about long term
    - *Response:* We have been thinking about GNDS and it's more robust formalism for cross correlations, **looking for community input** as to what's needed in a final
  - Do you have an estimate for developing covariance between data points from thermal to 500 keV.
    - *Response:* Because our values are different from ENDF, we are still looking into adjusting parameters and then use integral measurements to get feedback on
  - Is total kinetic energy an adjustable input?
    - *Response:* Yes, it's a fission fragment tunable parameter. Use fission nubar to lock down and provide more constraints on TKE because experimental TKE has large variance.
  - (Zerkle) What energy mesh do you expect to have the fission product yields at? Will this break the interpolation rule?
    - *Response:* We are looking for every 1 MeV from 0 – 20 MeV, still looking onto gridding format to avoid MCNP interpolation issues. Lin-log, still being explored, still needs to be weighed against final size weight.
  - (Andrew Holcomb) Have you compared your FPY results to those done for JEFF by the CEA? I think right now they have only finished FPY for neutron-induced fission of ^{235}U but they have computed the correlations as well, it would be great to do a cross comparison between their results and your results if possible

- *Response*: Yes, I agree we can discuss.
- (Talou) Yes, absolutely. There is also the IAEA CRP on FPY which will aim at such comparisons.
- (Holocomb) Precisely. Just wanted to make sure everyone is aware of all the great, exciting work being done! **Cross comparisons are invaluable at catching problems before they make their way into a released library.**

- **DISCUSSION:**
  - **Covariance format *** discussed further at the end of session (look below) *****
    - Create an MF38 format (like MF35) for covariances; move FPY uncertainties out of MF8 into MF38 only
    - Extend the MF8 format to include correlations as well as uncertainties
    - (Dave) I do not like either of these options... we will have to reinvent the wheel so if it's desperately needed right now we can do it but if not, we should think long term
    - Main format user is ORNL and we should get input from them
      - (Doro) new covariances in GNDS can be processed by ORNL... don't think NJOY can but the same would be nice for resonance covariances

Analysis of ^{235}U and ^{239,241}Pu delayed electron and gamma spectra measured by J.K. Dickens et al.

Speaker: Alejandro Sonzogni (NNDC - BNL)

Overview: A bookshelf in the NNDC research library collapsed and the NNDC found three reports detailing gamma and electron spectrum measured in the 1970s at ORNL using reactor irradiated foils measured from rabbit system. This is the only data set to provide measurements for times shorted less than 20 seconds. Dickens also measured antineutrino data from ^{235}U which agrees quite well with 2011 measurement by Huber. Delayed electron data from ^{235}U irradiations suggest that ^{92}Rb and ^{96}Y contributions are too large. Fortunately, the decay data is well known and independent fission yields and were therefore adjusted to match the data. For ^{101}Tc, ^{94}Y was adjusted against short, medium, and long fission yields. Long irradiation time gammas were predicted better than short irradiation times with the issue being the gamma detection method. Work is underway to adjust fission yields for 10 isotopes most of which are short lived.

Discussion Items:

- **ACTION**:
  - Summing-free singles gamma spectra to account for shorter irradiations and counting times needed
    - This was communicated to the main experimental groups & DNP
  - Data in EXFOR
- **QUESTION**:
  - (Zerkle) Where were foils irradiated and how long did rabbit transfer take?
    - *Response:* Irradiation time 1 second, delay time is 1.7s and counting time 110+s
    - Provides good measurement of short-lived fission product yields
  - (Toshihiko) Are there issues with modeling done with CGM that makes its way into ENDF? If there is, let Toshihiko know.

- (Jordan McDonnell) What is the magnitude of your adjustments? Could we compare your adjusted yields to Amy Lovell's results?
  - *Response:* Large adjustments around 50% for things like Cesium and Rb, could have issues with short lived isomers when FPs are outside the valley of stability. Data will be distributed on EXFOR shortly.

Experimental FY compilation and decay data corrections

Speaker: Andrea Mattera (BNL)

Overview: The current status of fission yield compilation is to collect, compile and correct experimental data for: ^{238}U(n,f), ^{241}Pu(n,f), ^{239}Pu(n,f), ^{235}U(n,f). Additionally, there is work underway to collect, compile, correct and evaluate Isomeric Yield Ratios from all fissioning systems (sf, n-, g-, p-induced). Starting from NSR database (expected to be more complete than EXFOR compilation), data is imported from JSON-FY into database and implement correction for decay data. JSON file types allow comments, secondary corrections, etc. to be and read along with data in file. The decay data correction is around 20-30% of EXFOR entries which contain information on decay data used in the experiment. It is necessary to update decay data with latest values to auto-scale values based on well-known intensities. Dependencies are used to identify outliers or issues with experimental data. Finally, work is ongoing to document and report EXFOR compilation issues, outliers, changes to uncertainties/experimental values and possibly unreliable measurements. Compiled over 538 independent isomeric yield ratios from 39 compound nuclei. This is 5x the amount of data available to Madland and England when they developed models, so new improvement in predicative capabilities can be made. This work is looking to validate with Amy Lovell's models and then perform additional experimental activities.

Discussion Items:

- **QUESTION**
  - (Marco) Will the corrections work be in EXFOR or parallel database?
    - *Response*: when we update the value of the yield it is not included in EXFOR – separate repository
  - (Kawano) Is there a document to keep information?
    - *Response:* data is stored in JSON; individual technical reports are published by BNL.
    - (Talou) In response to the last question about EXFOR, the WPEC SG50 is working on this exact problem, building layers of curated experimental data on top of the EXFOR base layer. Check it out: https://www.oecd-nea.org/download/wpec/sg50/

Prediction of the initial conditions of fission fragments from microscopic theory - Possible consequences for Evaluations

Speaker: Nicolas Schunck (Lawrence Livermore National Laboratory)

Overview: This work is looking to build a theoretical bridge between cross sections and fission product yields by developing microscopic theory of scission process. There is a need to input the mode

of nuclear forces and quantum many-body methods. Cumulative fission product yields are the result of a complex chain of events so the knowledge of initial conditions at scission is key to simulate the decays. No experimental measurements are possible at scission so we rely fully on theoretical models. LLNL uses a fundamental approach to fission theory based on nuclear density functional theory to provide initial conditions for fission fragments and uses an event generator (FREYA) to validate them. Under consideration are number of particles in fission fragments, spin distributions and fission of odd-mass nuclei. LLNL effort is focused on providing guidance for the evaluation of FPY by developing and applying microscopic models for the initial conditions of fission fragments.

Discussion Items:

- **QUESTION**:
    - (Talou) Any idea on how to expand your method to study the dependence of your calculated Y(Z,A) on the entrance channel, e.g., photofission vs (n,f) vs spontaneous fission?
        - Response (Nicolas): it is possible to take potential energies we have and project them, then calculate yield
        - (Gregory Potel) Concerning Patrick's first question ((g,f) vs (n,f)). Wouldn't be enough to compute the spin distribution induced by the incident gamma, instead that by the neutron as we do now, and invoke Bohr's hypothesis (decay independent of formation) from there?
        - (Nicolas) Yes, we should do what you propose. There will be a difference, and that difference may also depend on which target nucleus we consider.
        - (Talou) Regarding Gregory's comment, yes indeed, you would want to down select the particular (J,pi) states of your compound nucleus formed by either entrance channel. Bohr's independence hypothesis is what you would want to test, not assume. If you obtain different Y(Z,A) for different formation channels, then you should see differences in prompt observables. As for Nicolas's comment, yes, those thermal effects should also be important. Even after relaxation, most fragments have a non-zero ground-state deformation. Seems complicated…
        - (Gregory Potel) Good point about testing, not assuming, Bohr's hypothesis. A way to go beyond considering only differences in spin for (n,g) vs (n,f) could be to consider pre-equilibrium processes in both cases "before" we "look" at fission. Those are different for gamma and neutrons and go beyond Bohr's hypothesis. And we know how to calculate them…
    - (Talou) The fragments at scission are usually more deformed than in their ground-state indeed, but decay codes like FREYA or CGMF start at the point where the two fragments are well separated and have relaxed to their ground state shape. What would be the impact on the residual spin distribution in the fragments?
        - Response (Nicolas): if the fragments have relaxed to the g.s. shape, that deformation energy must have been converted into some "thermal" excitation energy of the fragments (since by definition, particle emission has not started yet). So on the one hand, deformation effects - which broaden the spin distribution - are much lower, but thermal effects - which also broaden these distributions - are larger: I am curious to see how this plays out. Also, results from TDDFT suggest that fragments exhibit collective vibrations after they are formed: these could also affect all these calculations.

- (Ian Thompson) Do you have experimental evidence of the spin dependency of fission products?
  - *Response:* Looking into it but that's difficult to answer. Yields are taken as empirical functions so we don't see physical evidence
  - (Ian Thompson) resonances have different spins (based on an old measurement)
- (Kawano) Are you looking at neutron angular momentum being applied to whole body calculations of the compound?
  - *Response:* to do this we would need to break symmetry argument. Start from J and go to K, limitations of current model prevent access to K.
- (Jordan McDonnell)
  - We are doing evaluations for different values with uncertainties on the predictions

Preliminary Study of Photo-nuclear Fission Product Yield Evaluation

Speaker: Toshihiko Kawano (Los Alamos National Laboratory)

Overview: The IAEA 2019 Photonuclear data library includes both the photon strength function and photonuclear data library and there are some inconsistencies with ENDF. The major actinide data was evaluated (and improved) by N. Iwamoto using CCONE code up to 200 MeV. There exists a missing section reported by users for photo-fission gamma-ray production. The fission gamma-ray multiplicities are much lower than expected and previously reported. The idea is to apply a technique to produce neutron induced gamma-rays. CoH3/BeoH has been extended to photo-induced multi-chance fission. Evaluation of gamma-ray production from photo-nuclear fission needs FPYs for gamma-ray induced fission. The average number of prompt fission neutron data were fitted by tuning the total kinetic energy (TKE). The average number of delayed neutrons includes the multi-chance fission effect and agrees with the evaluation. Prompt fission gamma-ray energy spectra were also calculated and isotopes can be identified. More experimental data will be useful to benchmark these calculations. Bremsstrahlung data is preliminarily compared to cumulative photo-fission mass yields and it seems reasonable.

Discussion Items:

- **ACTION**:
  - Experimental data!!!!
- **QUESTION**:
  - (Dave Brown) does this mean we get a new sub library?
    - (Alejandro) It would be helpful if this data was available in a sub library.
    - (Kawano) We would need a new covariance format.
  - (Dan Roubtsov) is it possible to separate fission gamma ray and capture gamma rays involved in reactions?
    - *Response:* Yes, you can separate, need reformatting in IAEA codes.

Fission Product Yields Formatting Discussion

Speaker: Amy Lovell

Overview: Two formatting options are available.

1) Create MF38 format much like MF35 for covariances, move FPY uncertainties out of MF8 to MF38. E
2) Extend the MF8 format to include correlations as well as uncertainties. Cross correlations between incident energies not included.

Discussion Items:

- **DISCUSSION**:
    - (Alejandro) Some people have not heard of GNDS and do not use some of the processing codes. If you need to compare 8.0 and 8.1 and they are in completely different formats, some users will not be happy. It may be useful to maintain the current format and a correlation matrix.
        - It would also be nice to have the mass yields that were used, since they cannot be reconstructed from the file.
        - This could be more difficult to go from pre- to post-neutron.
    - (Doro) All formats will require changes in the processing codes. All codes can read the current GNDS format so the impact to processing codes will be much less.
        - ENDF/B-8.1 is coming out in both ENDF-6 and GNDS formats.
    - (Dave Brown) What is the current status of the processing codes? What do the people who are writing the codes want to deal with?
        - (Nathan) NJOY can read GNDS but can't actually do anything with it – exclusively using GNDS will not be supported in NJOY initially.
    - Full covariance is already supported in GNDS.
    - (Talou) On FPY covariances, I don't understand the argument that GNDS is any better than ENDF in that case. I would echo Alejandro's remark that storing those covariances in GNDS only would be detrimental to various communities.
        - (Caleb Mattoon) we want to get away from truncating to 6 digits with GNDS and have better support for full covariances
            - (Holcomb) If you cannot accurately represent the correlation matrix correctly, you are missing information. GNDS will allow you to store this information correctly?
        - (Talou) Full Double float vs. Fortran a-11 formatting. Need more than 6 decimal points.
    - (Denise) Large covariances for first chance fission
        - Need to look at this still... not sure how covariances change across incident energy, first chance fission is not a huge problem. The covariances might change more rapidly with multi-chance fission.
            - There are applications at both low and high energies that will need to be worried about.
    - (Denise) what are the energies? (Low energies are not a problem) Why do the uncertainties need to be taken out of File 8?
        - It is a safer option? We hope if full correlations will be included, people will use them.
        - (Doro) we need changes to all of the codes that are using the data. (I.e. Origin, Cinder, etc. Users)

    - (Zerkle) keeping the uncertainties in File 8 gives a lot of time to transition to the new formats.
- (Jason Thompson) Why does the first option need to move uncertainties?
    - (Doro) Because we don't want to store the information in two places in case someone forgets to update both. The goal is to have uniformity and standardization.
- Energy grids – lin-lin vs. Lin-log, need data to see which ones will be useful for reactor calculations.

DOE Town Hall and NSAC Nuclear Data Charge

Chair: David Brown (BNL)
Date: Thursday, November 3, 2022

NSAC Nuclear Data Charge

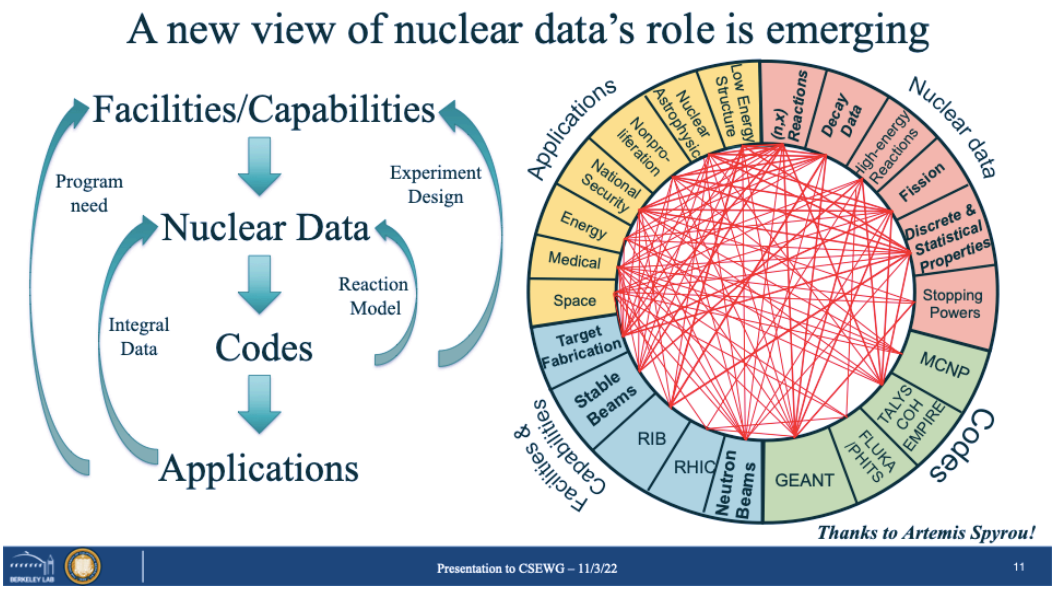
Speaker: Lee Bernstein (LLNL/UCB)

Overview: Nuclear Science Advisory Committee (NSAC) is working on a call to submit a long-range plan. A nuclear data charge was issued to the full nuclear physics community and a large paper was compiled. The DOE/NSF NSAC has been asked to prepare a pair of reports on nuclear data. The first part of the charge was to assess USDNP status which included assessing and documenting recent achievements and their impact, survey current and future federal/non-federal needs for reliable, accurate, secure and accessible nuclear data and assess the role, competitiveness and importance of the USDNP in an international context. A team of nuclear data users and experts in fields that aren't typically nuclear data providers but are heavy users was assembled and they identified cross cutting needs.

Cross Cutting Needs

- Workforce development including training and *retention* - we are resource limited
- Ongoing fission evaluations - FPY should not be once every 30 years - **structure and reactions data**
- Accelerated decay data evaluations - need resources to improve decay data as it is available
- Improved reaction modeling via extended nuclear structure data evaluation - not just fitting critical experiments - want the correct physics - RIPL is here but we need more
- (n,x) data from thermal to 20 MeV (including structure, y-ray production)
- High energy reactions and stopping powers - moving beyond 20 MeV to be relevant to this community

New view of Nuclear Data's Role



The second part of the charge is to provide recommendations for maintaining effective stewardship of nuclear data including identifying and prioritizing the most compelling opportunities to enhance and advance NP stewardship of nuclear data, train and retain the workforce and access needs for facilities and instrumentation, cross-cutting opportunities with other federal programs and potentially mutually beneficial interactions with other domestic and international stakeholders.

Discussion Items:

- **QUESTION**:
  - (Mark Paris) Fusion was noticeably absent in Phase I, suggest talking to the **ICF** personnel at LLNL.
    - (Lee) This should be fixed immediately, and please reach out to LLNL. We are working on gaining their input, need more than inertial confinement fusion. **Magnetic confinement fusion** needs to be addressed in addition to **materials damage** also requires significant attention.

Town Hall Process

Speaker: Ramona Vogt (LLNL and UC Davis)

Overview: Every 5-8 years, the funding agencies (DOE and NSF) issue a charge to the Nuclear Science Advisory Committee (NSAC) to produce a Long-Range Plan. The last previous charge was in 2014, the most recent charge was delivered to NSAC in July 2022 and is expected to be completed by October 2023. The process determines the priorities for US nuclear physics during the next 5–8-year period by agreeing on a number of recommendations and initiatives. USNDP/CSEWG activities are funded under US DOE NP. Several budgetary considerations: constant or modest (2%) growth is lower bound but upper bound could be new funding from the CHIPS act for the next 5 years if a compelling case is made. In general, great opportunities are possible with a good LRP so the community needs to

come together to produce an equitable, inclusive document in the broadest possible sense. **We need to work together and respect our community.**

Requesting support:

- Participate in the town halls
- Give your input to the ND subcommittee and the LRP writing committee
- Support the plan developed by the whole community
- Nuclear data will be an integral part of the LRP for the first time – this is a BIG DEAL!
- We have a great opportunity to expand and grow nuclear data in new directions
- We need to show that the data community is strong, inclusive, and ready to take on and meet new challenges

Subcommittees created:

- QCD
- Fundamental Symmetries
- Nuclear Structure & Nuclear Astrophysics
- Workforce Development (includes education and DEI)
- Applications
- International Context
- Crosscutting/interdisciplinary scientific opportunities (e.g., QIS, Accelerator Science, Computing)
- Impact and synergies with other fields (e.g., High Energy Physics)
- Budget
- Theory

The writing is going to commence over this next year (will include a 5-day resolution meeting) with the goal for the draft to be completed by Oct 2023. Three Town Halls are planned for the coming year, seeking strong nuclear data community participation. The inclusion of nuclear data in the long-range plan is exciting and positive. This opportunity needs to be seized to secure federal investments in nuclear data, collaboration with new agencies, and continued growth of the community.

Discussion Items:

- **DISCUSSION**:
    - (Lee) Inclusion is very important and we need to send Lee information
    - (Michael Smith) we have an opportunity to get our point across but we won't have room in the report for what we want in the next 10 years of nuclear data. **We need to distinguish what is the purpose of these two documents.**
        - All townhalls are making white papers
        - Document will be stand alone
        - It won't have a lot of detail. It's most important that Washington sees that this is a good field and they should fund this work
        - It will give valuable information to the LRP as well
    - (Zerkle) energy range discussed is not applicable to many of us in the room
        - New ORELA would have the biggest impact from science to the applications community

        - (Dave Brown) it's good to talk about it in this room because not many of us are funded directly by science and we are not accustomed to the openness and transparency of the work
    - (Lee) **Let's have another working group to focus on collaborative efforts between DOE science and CSEWG participants**

Evaluation Committee [Charged Particles]

Chair: Marco Pigni (ORNL)
Date: Thursday, November 3, 2022

(α,n) studies at the University of Notre Dame and Ohio University

Speaker: James deBoer (University of Notre Dame)

Overview: IAEA workshops highlighted R-matrix code needs for charged particle interactions. New HeBGB detector sacrifices low neutron energy efficiency for a relatively flat neutron detection efficiency. The HeBGB detector is capable of measuring (α,n) reactions to high fidelity in the high energy regime (1 - 10 MeV). The detector is not completely a 4π array so there is some dependency on the angular distribution of the reaction channel. The detector is capable of resolving discrepancies between international evaluations by providing superior data compared to past systems which produced older evaluations. The Notre Dame 5 MV single ended accelerator and ODeSA measured scattering angular distributions (18-point angle distributions) with 10 keV or smaller energy binning. Bayesian MC fitting is underway on the improved $^{13}C(n,\alpha)^{16}O$ to update the $^{16}O(n,\alpha)$. 2023 R-matrix workshop on methods and applications in Athen, OH in June 2023.

Discussion Items:

- **QUESTION**:
  - (Marco) What are your plans on Fluorine?
    - *Response:* We're looking at it and seeking funding to measure.
    - Are there any concerns with this type of measurement/sample?
      - Targets are challenging but we believe we can get a target that will provide good results. Need to avoid a stable fluoride material that won't degrade under beam fluence
    - Are there any proton emission issues and can you measure it?
      - *Response:* Yes, we can measure it but detection methods are completely different and need to be reworked.
  - What is the HeBGB detector efficiency?
    - Significant uncertainty in HeBGB detector which is primarily attributed to uncertainty in ^{252}Cf source used for energy calibration.
  - (Mark Paris) How does this measurement compare with previous measurements (one in particular - didn't catch the name)?
    - At the back angles we see larger disagreement compared to front angles, but more extensive analysis needed to conclude final comparison between the datasets

Candidate evaluation for $^{3}He + ^{4}He$ scattering from R-matrix theory

Speaker: Ian Thompson (LLNL)

Overview: Discussion of R-matrix framework and how to integrate into ENFD/B8 for (^{3}He, α). The goal of this work is to check the problems with EXFOR with respect to fitting data. Charged particle data

is a long way from being in EXFOR. The fitted R-matrix parameters will be included in MF2 using the LRF7 format. Brune basis can be used to transform energies to constrained energies where the peaks are located. The proton channel is predicted equally well with the R-matrix theory. Python codes were developed to take R-matrix and structure with GNDS code to test and check.

Discussion Items:

- **ACTION**:
  - More work for higher ^{1}H energies (^{1}H + ^{6}Li --> ^{4}He + ^{3}He reaction)
- **QUESTION**:
  - (Mark Paris) never finalized the normalizations
    - *Response:* read the paper to understand how to fit. Serious evaluation decisions need to be made for that.
    - (Mark) when parameters are available to download and plot to compare to data... where are we placing the normalization?
    - (Thompson) in GNDS we store the numbers and read them back. We should have a simplified form in the ENDF format (follow up with discussion with SG50)
  - (Vivian Dimitriou) we all read data and suggested/discussed normalizations for each measurement. Is there any room for improvement? What is the plan?
    - *Response:* Determine the discrepancies between different experiments and the next step is to decide which measurement will be accepted.
    - (Marco) when we align experiments and introduce shift, we don't have room in the model to fit the data appropriately
    - (Vivian) it will also be beneficial to compare to other evaluations... what is currently in ENDF?
      - ECPLs collection of data from LLNL (1-channel) collecting data rather than R-matrix fit, does not give angular distributions

Charged-particle sublibrary evaluations in multi-channel unitary R-matrix approach

Speaker: Mark Paris (LANL T-2)

Overview: Discuss R-matrix formalism and use the 5Li system charged particle sub library and issues to clarify. [Formats side note: encoded in MF2 in RRR for LRF7 (R-matrix limited – unlimited partitions of channels) In ND2007, Nancy Larson clarified that limited is going to allow wave functions that are not coulomb or free.] LANL has made the following contributions to evaluated libraries as part of the light element evaluation effort.

Projectile\Target	^{1}H	^{2}H	^{3}H	^{3}He	^{4}He	^{6}Li	^{7}Li
n	2020	VIII.0	VIII.0	VIII.0	VIII.0	2020	VIII.0
p	2020	VIII.0	VIII.0	VIII.0	2020	VIII.0	VIII.0
d		VIII.0	VIII.0	2020	VIII.0[a]	VIII.0	VIII.0
t			VIII.0	VIII.0	2020	VIII.0	TENDL09
$h(^{3}\mathrm{He})$				VIII.0	VIII.0	VIII.0	TENDL09
α					VIII.0	TENDL09	TENDL09
^{11}B (α+^{7}Li, α+^{7}Li*, t+^{8}Be, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)							
^{12}C (α+^{8}Be, p+^{11}B)							
^{13}C (n+^{12}C, n+^{12}C*)							
^{14}C (n+^{13}C)							
^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)							
^{16}O (g+^{16}O, α+^{12}C)							
^{17}O (n+^{16}O, α+^{13}C)							
^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)							

Local testing and comparisons are also made. Changes to D-^{3}He fixed up angular distributions. Continuing to add R-Matrix parameterization capabilities to NJOY is essential to accommodate new evaluations. More testing and contributions will be required to enhance NJOY to the required level for these LRF7 evaluations.

Discussion Items:

- **ACTION**:
  - Further testing required to understand why MF2 resonance parameters are not predicting correctly... think it's a formatting issue (NJOY test is buggy)
- **QUESTION**:
  - (Gustavo) phase 1 stores files, then merge request for phase 2, submitting evaluations can have attachments to the review
    - (Wim) LRF7 KRN4 cause some issues (Coulomb wave functions). We have done some verification work with neutrons, and we think that charged particle channels are the issue.
    - (Andrew Holcomb) We fixed some things in AMPX, looking at spin groups should/should not be included could also cause some difficulties, could add different backgrounds
  - (Marco) this is parameter from INDEN?
    - Yes, discussion on classic vs. relativistic parameters. Results are still classical and will be improved on going forward.
  - (Jonathan) **Can we do these –L evaluations now?** It was previously discouraged
    - (Dave) It's not clear from formatting committee. Will be discussed tomorrow.
    - (Mark) It's the evaluators choice when going around the formatting and processing codes.
    - (Ian Thompson) once you do point-wise reconstruction, you should not include R-matrix parameters
    - (Doro) GNDS format could make it difficult
    - **Conclusion: have point-wise AND R-matrix parameters submitted to CSEWG**

    - (Andrew Holcomb) even though it is not stated in the manual, the codes assume that the eliminated capture channel is always the first particle pair definition, followed by the elastic channel for LRF7
    - (Andrej Trkov) Using new features like the boundary conditions in ENDF would call for a "code verification exercise" to see that they all produce the same cross sections. Can you also provide an example evaluation for code checking?
        - Marco was going back and forth with everyone, trying to validate the different processing codes.
        - Andrej, Mark and Marco are all on the same page and will do this
- **RESOLVED**:
    - Begin the validation test suite to be shared across processing codes to address charge particle R-matrix.
- **DISCUSSION**:
    - Going through line by line – there are issues that were not applicable to charged particle – so they changed some of the language -
    - LRF7 is currently the desired format (backward compatibility) there might be redundancies – want to revisit this next CSEWG

WANDA Planning

Chair: Bruce Pierson (PNNL), Amy Lovell (LANL T-2)
Date: Thursday, November 3, 2022

WANDA will be held in Washington D.C. during the week of February 27th-March 2nd 2023 (in-person only). Indico website is open, other registration page will be released soon.

Date/Time	Topic
Feb. 27th, 2023 0800-1200	Plenary • Program Manager Discussions • Nuclear Data Pipeline Review
Feb. 27th, 2023 1300-1700	Gamma Strength Functions & Level Densities
Feb. 28th, 2023 0800-1700	Fission Yields, where we were, are, and headed/Theory, Evaluation, Experiments
Mar. 1st, 2023 0800-1200	Isotope Programs Session
Mar. 1st, 2023 1300-1800	Nuclear Data Processing & Preservation
Mar. 2nd, 2023 0800-1200	Active Projects Overview
Mar. 2nd, 2023 1300-1700	Session Outcomes Closing Discussion

Highlight of WANDA is need based talks from nuclear data users from all aspects of the industry and sciences. General procedure is that nuclear data creators/processors moderate talks from the users themselves to highlight pain points and future needs.

Sponsors: NNL, NASA, NA22, NRC, NA11, NCSP

- **Gamma Strength Functions/Level Densities** (Stephanie Lyons [PNNL] & Gencho Rusev [LANL])
  - Brief discussion of current theory and definitions, level densities and gamma strengths impact the understanding and development of neutron and charge particle data. Leverage theory to narrow down the distributions on levels.
  - Speakers: Steve Grimes, Ann-Cecillie Larson/Magne Guttormsen, Mattis Wiedeking, Lee Bernstein, Shaun Liddick, Cecilia Larson (?)
  - Topics: (Cathy) Audience is not nuclear data people but users of data, suggest having Lee Bernstein talk about why we care about level densities, how it impacts all nuclear data, theory & evals. Again, avoid discussion on the process but more the needs, (Mike Herman) getting these values are important but how they are implemented is another story.

- **Fission Yields** (Jason Harke) harke2@llnl.gov

- Speakers: Guy Savard, Andrea Mattera/Alejandro (BNL), Matt Gooden, Toshihiko Kawano, Patrick Talou, Gencho Rusev, Roberto Capote, r-process: Nicole Vassh for this, ML/AI applications to r-process: Matt Mumpower, Amy Lovell (covariances), Robert Mills,
- the first authors on the most recent fission yield modelling papers are Goriely, Mumpower, Vassh, and Holmbeck
- Topics: Semi-integral measurements/R-values, validation, processing, covariances, (M. Zerkle and B. Little) suggest marketing the rabbit system on GODIVA4.

- **Isotope Programs Session** (Etienne Vermeulen (LANL), Andrew Voyles (LBNL/LLNL))
  - Need one more chair from neutrons – ORNL?
  - Speakers: Dmitri Medvedev (TREND), Jerry Nolen (ANL) , Roy Copping? (ORNL), Jon Engle, (UWis), Greg Moffit (UWash), Roger Howell (Rutgers), Suzy Lapi (UAB), Lauren McIntosh (TAMU), Staff member from FRIB for isotope harvesting, Alex Hermanne (aherman@vub.be), Prof Qaim, Justin Griswold (ORNL)
  - Topics:
    - Status update and needs from 2018 speakers
    - Targetry, postpone till next year
    - Improvements to measurement robustness, where are we headed?
    - Stable isotope production (important for this community) - specifically what, how much, availability and when

- **Nuclear Data Processing and Preservation** [Libby Ricard-McCutchan (BNL) and Nathan Gibson (LANL) ngibson@lanl.gov
  - Two – 2.5 hr sessions, need 30 minutes for general Q&A.
  - Speakers: Reps from all processing codes, each talking about where are you going with code. People pushing advance architectures (Paul Romano), LANL\LLNL for deterministic transport. Pat Griffin for damage cross sections. Fusion material speaker. Caleb Matoon regarding GNDS.
    - (Keith) someone from OSTI or our DOE SC working group on data can speak if you think some general info on these topics is useful – agreed from Libby
  - Topics:
    - **Future** of nuclear data processing!
    - New processing requirements for FPY.
    - Rising HPCs and CPU architectures allows for new capabilities for processing codes which should be optimized
    - Processing beyond neutron transport
      - Covariance, heating, damage cross sections, fusion materials damage, incident charged particles/photons, etc.
    - Processing covariance with GNDS should be mentioned but it shouldn't take up a considerable portion of the talk.
    - More efforts to document analysis of experimental data to allow for better reproducibility of said data.
      - Specifically need to document data reduction processes, assumptions, error fixes, data interpretation, etc.
      - Preservation of raw data with information about calibrations, geometries, instrumentations, etc.

        - Get ideas and suggestions of how to curate, preserve and eventually share the data.
        - Learn from people who have already done it well
        - Processing codes should also be stored so the results can be reproduced
    - (Amanda Lewis) Go to communities to find how they get their data – running MCNP without thinking or EXFOR but not really knowing how to use it.
    - (Jesse Brown) Feedback from community about what we mean by "data".
        - Cross section is standard but something like count rates or other raw data can be useful
        - What physics data should be stored? This can be very experimentally specific and highly variant.
        - (Keith) Good point on "what is data". This is also being discussed at SC. Raw, processed, also any workflows
    - (Denise) Include evaluators in the discussions about what should be stored
        - Code/models developed by grad students and even readme files could be lacking in terms of level of development/documentation
    - (Roberto) - Reinforcing that we need ***all*** parts of the experiment documented for accurate reproducibility
    - Has to be benefit to adding this reproducibility/documentation step so it's not a burden but rather a beneficial step in their research. Automatic Co-authorship on using data?
    - Data publishing needs to be included in the experiment pipeline. Just because results are achieved, the project is NOT DONE.
    - Boris – Sometimes only a partial data set is released, can journals support data preservation?
    - (Keith Jankowski) Discussions are also underway internally about how to capture data management costs. As is, the standard forms don't have a spot for it but it's useful (critical?) to know. We also have updated guidance for data management plans to help both proposers and reviewers in addressing DMP related content. https://science.osti.gov/Funding-Opportunities/Digital-Data-Management
    - (Zerkle) ask program managers how they plan to implement new open data sharing requirements
        - Roberto – need to sort out what we really want besides cross sections
    - (Lovell) the steps forward can include looking to the scope of the issues, form working groups and have further discussions
- Active Projects Overview
    - Topics: (Keith Jankowski) This project list looks mostly accurate still, but I'll send you the updates for the new starts this year from NP (5)
    - (Denise) New FOAs
    - **This list needs to be distributed – request by audience**
    - Cathy will work with Bruce on this

Poster Session Wednesday night of reception – student posters, focus on mentorship and making connections

Todd Bredeweg – suggest job board/positing at minimum

Formats and Processing

Chair: Doro Wiarda (ORNL) and Mike Dunn (Spectra Tech.)
Date: Friday, November 4, 2022

Welcome!

ENDF manual changes and Format Change Discussions

Speaker: David Brown (NNDC, Brookhaven National Laboratory)

Overview: Good Morning!
Manual Changes: Only two changes were made so far to the ENDF manual this FY.
New changes to appendix D for all things resonance parameters with the goal of updating for R-matrix limited. There are 24 Open issues, 3 error/typos - all TSL issues. MAT number seems to be an issue going forward, need to develop general rules instead of just choosing numbers. Action items listed, request everyone check status of their action items and try to resolve any issues/work to be done (See slides from talk). Further discussion regarding the status of other proposals (URR interpolations, MF4/5 changes, etc).

Discussion Items:

- **ACTION**:
  - Create a task force committee to solve material classification problem (limited range of numbers available)
    - Zerkle (NNL TSL), Wim (NJOY), Doro (SCALE), Bret (FUDGE)
  - Call for volunteers to help resolve improvement/requests
  - Provisionally accepted resonance-related proposals:
    - Brune (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/113) – action on **Marco, Ian**
    - R_ext (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/101) – action on **Wim, Jesse**
    - KRL (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/103) – action on **Mark, Ian**
  - Provisionally accepted IRDFF-related proposals:
    - MF10 (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/107) – action on **Andrej, Dave**
    - W (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/138) – action on **Andrej, Dave**
  - Provisionally accepted Kalbach-Mann proposal:
    - d breakup (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/112) – action on **Arjan, Dave**
  - Forgotten proposals:
    - Temp (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/106) – submitter is **Andrej**
    - MT's (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/102) – submitter is **Andrej**

- Unexpectedly hard proposal:
  - URR (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/105) – submitter is **Andrej** This should be easy, but we keep going around and around
    - Proposal by the manual – it should say interpolate on parameters and not the cross section.
    - Table this for now – keep discussion open
- Ones maybe we should just drop?
  - MF4/5 (https://git.nndc.bnl.gov/endf/format/endf6man/-/issues/92) – submitter is **Andrej** Requires information not present in ENDF files to make practical.
    - (Caleb Mattoon) Thinks we already have files that do this
    - (Dave Brown) but it can be inconsistent and not usable.
    - (Wim) MF6 – does not include 2 body kinematics so would need a new format.
    - (Andrej) MT 261 is used in spectra files in IRDFF - The request was only to reserve the MT number for dosimetry purposes - Do we assume that MF12,14 is allowed in two-body kinematics is prescribed in MF=6? I don't see that MF=6 gives any additional information

- **QUESTION**:
  - Each library will have its own list and material assignments
    - This has been resolved in JEFF and we should adopt the strategy
  - Trkov – if we do File 6, do we keep all of the information that is missing from files 4/5? Cannot handle gamma cascade of residual after the compound state.
    - All the info about both from both particles is kept in MF6, except:
      - No mass of the residual is kept, so there is not ability to handle the gamma cascade after the compound nucleus is formed.
- **RESOLVED**:
  - Transfer two body kinematics physics proposal for MF4/5 to law 4 in MF6
    - Keep action item open (explore with GNDS)
- **DISCUSSION**:
  - Lots of materials for TSLs – make it a separate document instead of in the appendix – TSL file has the number encoded
    - Up to 999 materials – Zerkle thinks there is not enough digits
      - In practice only 300-500 materials will be supported with a unique ID, this needs to be solved in the near future.
      - SCALE is only limited by size of integer, NJOY limited to 9999
        - NJOY people say that it is limited to 9999 (from ENDF).
  - Lots of open issues for improvement – primary gamma confusion can be turned into a full format proposal (Bret Beck)

TSL Concerns: isotopic evaluations for fuels

Speaker: Chris Chapman (Oak Ridge National Laboratory)

Overview: ORNL has discovered discrepant issues with how TSLs are handled between processing codes and transport codes. MT2/4 files have some inconsistent definitions for number of scattering atoms between incoherent inelastic/elastic scattering. Different processing codes handle these issues in different ways so it would be preferred to automate corrections to reduce the possibility of user error.

The proposed (but not an official proposal) solution is to include a generalized header file for the ENDF-format TSL files, that contain pertinent information for the scattering atoms (number of scattering atoms in molecule, and the isotopic distribution within the scattering atom). This should not be a significant change. This issue is open for discussion.

Discussion Items:

- **QUESTION**:
  - Is this something the community would like? The issues are not present in GNDS.
  - How should checking codes be changed to account for potential duplicate information?
  - What other information should be included?
  - Would density information also be conveyed?
    - (Zerkle) Some materials like graphite are weird. There are lots of processing parameters that can be codified and interpolated against.
      - (Chapman) This is something that can be done by an application code.
      - (Beck) I would prefer that all of this information can be parsed by any application code, there should be as much information present as possible.
        - (Zerkle) TSLs are very dependent on material structure, unsure if this should be in the ENDF file.
        - (Chapman) Is the crystal structure really that important?
          - (Zerkle) It is.
          - (Chapman) We could include this information, I am unsure if this information can easily be included.
- **DISCUSSION**:
  - Use of MF7 MT1 (since this is currently unused) as a generalized header for TSL files (similar to MF1 MT451 in traditional ENDF-6 files).
  - (Skip Kahler) NJOY requires user input for the number of primary atoms. It is available in modern TSL evaluations but was not provided in legacy (ENDF/B-III) evaluations, i.e., what you call "self-consistent N_atom" was not defined in ENDF/B-III.
    - (Wim) User still needs to give it, not checked against within the file.
    - (Zerkle) Most processing codes don't really support these mixed moderators from ENDF/B-III anyway so just leave them.
  - (Dan Roubtsov) We should take it seriously and fully support.
  - (Wormald) Disordered alloy theory only affects the data on MT=2 for coherent elastic scattering, which is always dependent on the isotopic composition anyways.
    - (Chapman) Yes that is correct. If we want to reconstruct the distribution of the mixed-alloy theory how many parameters would you need? This is more work for processing codes which is not something people want.
  - (Zerkle) File 7 is designed for elemental evaluations so moving to isotopic will require new capabilities.
    - Issues on properly treating coherent scattering.

- (Andrew Holcomb) - Thermal resonances in $^{235/238}$U will now affect scattering. Very important topic of breaking down TSL on per isotope basis of the material to ensure no misassigning of resonances to other isotopes.

TSL Concerns: TSL GNDS

Speaker: Caleb Mattoon (Lawrence Livermore National Lab)

Overview: Separate containers of TSLs have been merged into a single elastic term (coherent/incoherent can be split). GNDS will support storing crystal structure, incoherent inelastic evaluations, and more. Isotopics and blending between thermal and 'fast' neutron regions is important and challenge i.e. going from ZrH thermal to isotopic evaluations of Zr above thermal cutoff. Currently, all mixed moderator/isotopic moderator are treated equally and need to be checked against MF1 to see what's going on. When designing GNDS-2.0, S(α,β) are assumed to be on a linear interpolation grid.

Discussion Items:

- **QUESTION**:
  - Should users be interpolating S with respect to temperature?
- **DISCUSSION**:
  - The coherent inelastic terms are separable, so should they be stored as separate or together?
    - (Kemal) There is no need to separate, when we calculate, they are calculated as one.
      - You have only one inelastic component – (Zerkle) some codes have already been separated
        - (Kemal) You don't gain much by separating them out.
        - (Dan Roubtsov) I believe that having them separating them out is better for future evaluators because there is a need to store each component separately than the sum. Polarized neutron beam experiments can be used to validate the theory.
        - (Zerkle) This problem comes in with solids, Be and Aluminum - not enough information known at this time to make a formatting/processing decision
        - (Wormald) Processing codes like NJOY/NDEX often ignore the log-lin interpolation for S(α,β) as a function of β and use quadratic instead
  - There is a need to switch to standard incoherent neutron evaluations for energies or temperatures outside of TSL evaluations.
  - (Zerkle) NJOY would abort if we combined 3 components in MT4 for TSL evaluations.
    - NJOY limitations exist, Wim does not know if this problem is currently fixed.
    - (Zerkle) People complain about how big the files are so we remove information and then people complain that information is missing.
    - Mixed moderators SHOULD NOT be produced anymore, need isotopic evaluations, include in appendix.
  - JENDL-5 is interpolating S w/ respect for T, do we think that this should be supported? Does the physics support this?

- Ambiguities in interpolation schemes/quantities to be interpolated need to be clarified in GNDS.

URR Concerns: Covariances in the URR

Speaker: Dorothea Wiarda (ORNL)

Overview: There were discussions of limitations in the URR, and the purpose of the talk is to facilitate discussion with a focus on covariance information (*not a proposal*). Inputs were taken from Amanda Lewis and Devin Barry from NNL. Some limitations are resolved in GNDS. There are various solutions that arise:

Solution 1: No format change is necessary. We would add the generated covariance from SAMMY (or other MF33 generator) to MF33 – this is a grouped energy solution.

Solution 2: No format change is necessary. We would give covariances for each energy range, which might work in File 32. This cannot be done in MF2, so there is a need to add to MF32, but this approach would not allow for quantification of cross correlations.

Solution 3: Format changes would be needed. We would change the format to allow the full covariance for all resonance parameters and all energies.

Solution 4: Add covariances with respect to the resonance. parameter into GNDS and covariances with respect to cross section in File 32 in the ENDF file.

Covariances with respect to average cross section are sufficient for transport codes. But is it more physically accurate to add covariance to background cross section in MF3 or fluctuation parameters given in MF2? The last sticking point is reproducibility; processing codes, transport codes, and evaluators are all looking for different levels of fidelity. Consistency across file formats also (ENDF, GNDS) will be required.

Discussion Items:

- **DISCUSSION**:
  - What size of the covariance are we talking about?
    - (Doro)- Not very large, its only 5 parameters and it not insurmountable
    - (Dunn) - In the past ORNL has provided file 32 and made the file huge
    - (Doro)-Evaluator will always have to choose the group size and energy points.
  - Might be good to store covariance information but store in GNDS only, which is good enough for transport codes.
  - (Caleb) The new format would have an energy dependent covariance matrix.

GNDS Overview Plus New Developments

Speaker: Caleb Mattoon (Lawrence Livermore National Lab)

Overview: Major changes are coming to the GNDS2.0 format, and a publication will be coming soon. Primary gammas from capture are being studied with the GRIN project. These changes add xsdir file-like capability to GNDS. ENDF/B-VIII.0 is available as 850 Mb tar.gz file, which contains all sub-libraries, including reconstructed resonance. GNDS is currently supported by: Fudge (full), AMPX (nearly full for

1.9), NECP-Atlas (partial for 1.9), NJOY (started), FRENDY/GALILEE(Planned), GIDI+, MECURY, etc. FUDGE is a general toolkit for generating, testing, plotting and modifying ND as well as translating to other formats. What is the benefit of changing formats? We have the experience of doing this at LLNL, with a lot of effort to change codes. If there are a lot of codes to be updated, it will be a big effort. GNDS is a more robust and simple format for those unfamiliar with complex ENDF-6 format. The top priority is to abstract nodes and JSON schema adoption, then reducing redundancy, revisit PoPs and then clean up uncertainties.

Discussion Items:

- **ACTION**:
  - Looking for people to join EG-GNDS meeting if you're interested in contributing
- **QUESTION**:
  - Is the idea to move from XML to JSON in the future?
    - No, the idea is that the format specification is in JSON but we want to give users the ability to store data however they want. Need some sort of internal memory storage, can use JSON/XML schema. Big focus is storing and handling meta-data (attributes).
  - JSON schema is not fully supported yet – will follow up

FUDGE and GIDI++

Speaker: Bret Beck (LLNL), Caleb Mattoon (Lawrence Livermore National Lab)

Overview: Everything is currently up on GitHub, FUDGE is wrapped in a set of python modules which can process, modify, and plot data. FUDGE 6.0 was released in September 2022 with GNDS 2.0 support. The most recent update includes many updates giving users increased capabilities in the FUDGE API.

FUDGE includes Python scripts to help with some common nuclear data tasks including translation of ENDF-6 data into GNDS (endf2gnds.py /path/to/evaluation.endf evaluation.xml), running physics quality checks on GNDS data files (checkGNDS.py evaluation.xml), extracting outgoing spectra for specified products at specified projectile energies (energySpectrum.py evaluation.xml), processing data for Monte Carlo and/or deterministic transport (processProtare.py -mc -mg -up -t 293.6 -t 300 – temperature Unit K evaluation.xml proc.xml) and generation of ACE files (after Monte Carlo processing with processProtare.py) and more!

GIDI+ is a collection of (mainly) C++ APIs (i.e., sub-packages) for reading and sampling from GNDS data as needed by transport codes. Ardra (LLNL deterministic) and Mercury (LLNL MC) currently use GIDI+ and in the future so will GEANT4.

Discussion Items:

- **RESOLVED**:
  - Issues found in URR reconstruction have been addressed
- **DISCUSSION**:
  - (Gustavo) - I was happy to see you've been working on tutorials with FUDGE, really do need more tutorials

NJOY

Speaker: Wim Haeck (LANL)

Overview: This work is a report on the status of NJOY for ENDF/B-VIII.I. NJOY2016 is the production version of NJOY used at LANL – LANL recommends this as the version the community uses as well. NJOY2016.68 is most recent version (Sept 2022), which is currently available on GitHub. Mixed mode thermal scattering, improved photonuclear data all have impact to ACE formats, so MCNP will need to be updated. NJOY is always evolving and feedback about issues found is greatly encouraged. Mixed model elastic scattering and photonuclear ace files in ACER were both updated in NJOY2016.66 but the community will need MCNP6.3 to use these features. ENDFtk and ACEtk are being developed for manipulating ENDF and ACE file types. ENDFtk 1.0 will be released within the next few months. FY21 was focused on ACEtk development, incident neutron, charged particle, and photoatomic/photoneutron data to modify, plot, and recompile ACE. Work is continuing to modernize NJOY.

Discussion Items:

- **ACTION**:
  - Additional updates to ACE format and MCNP to process and utilize new nuclear data available in ENDF/B-VIII.I.
  - Process rest of ENDF/B-VIII.I library and sub libraries as they become available and validate results.
  - Continue with component-based modernization of NJOY (moving to modern C++ and python).
  - Add general R-Matrix and relativistic kinematics into resonance reconstruction theory.
- **QUESTION**:
  - (Gustavo) if you want a sneak peak of beta1, watch the phase 2 branch for all those ENDF files available to see. There are 5 in neutron, few in alpha, two in decay that were added just this week.
  - Dan Rou – Do you know how to communicate between MCNP/LANL, photoatomic library produced by EPR data?
    - We are going to implement EPR data to be read with ACE in order read and modify new ERP.
    - ERP data is processed outside of NJOY and loaded manually into MCNP.
  - Doro – For ACEtk can I now use it to covert the SCALE libraries to ACE?
    - Yes, it can be constructed backwards/forwards between SCALE and ACE.

AMPX

Speaker: Jordan McDonnell (UT-Battelle)

Overview: AMPX is now officially open source (https://code.ornl.gov/scale/code/scale-public). The AMPX GUI ExSite is available at (https://code.ornl.gov/scale/code/external/exsite). The low level GNDS classes are also available (https://code.ornl.gov/scale/code/external/gnds), with a branch (GNDS-2.0) supporting GNDS 2.0. TSL have an updated (finer) grid for scattering distributions, needed for cryogenic moderators. The AMPX team is looking to add separate MT for coherent, incoherent elastic scattering. SCALE6.3 should be released soon once export control allows the release. SCALE 7 will have several new multigroup libraries, mainly for use in HTGRs, sodium fast reactors. Niowave/NNSA/ORNL collaboration highlights need for SCALE to include photoneutron production. AMPX updated to now include ENDF/B-8 photonuclear data.

Discussion Items:

- **ACTION**:
  - There is a need to continue to incorporate GNDS2.0 into AMPX (GNDS1.9 fully supported).
  - Finalize short collision time subroutine for inclusion of improved thermal scattering angular gridding algorithm into future AMPX releases.
  - Continue to add capabilities to process photonuclear data to incorporate into future versions of SCALE.
- **QUESTION**:
  - How much parallelism is built into AMPX?
    - It is not put in at this time. Not as necessary as processing ENDF evaluations in parallel offers some speed-up.

Automated, Reproducible Data Processing, Verification, and Validation at the NEA

Speaker: Andrew Holcomb (Oak Ridge National Laboratory)

Overview: Automation to perform consistency checks and then process with several codes to different formats. These formats are then run through verification suites and finally validation suites (ICSBEP). The AMPX ExSite GUI was leveraged to automate input and verification inputs. This is implemented for testing with SCALE/AMPX and NJOY and MCNP/ Incorporation of other codes and more validation inputs are desired. Improvements are being made with a wholistic interpretation of nuclear data pipeline in mind to best meet the needs of the community. Integration with processing and validation of JEFF-4 is ongoing.

Discussion Items:

- **ACTION**:
  - Automatic processing for JANIS --> Nicholas processing system already implemented
  - Fully integrate AMPX processing and SCALE testing into validation and data processing efforts
- **QUESTION**:
  - (Andrej) Selection of benchmarks use DICE/WHISPER and perturbation techniques to find the most appropriate and go from there.
    - Yes, this will be done, still trying to figure out how to best select benchmarks for a given evaluation.
    - Please share any validation suites you have if any.
      - I've given over my benchmark suites and still have more but no one has used them/went missing for OECD.
  - (Arjan) I want validation on the spot if I update my evaluation. Could there be a system where new evaluations can be submitted as I go and run and directly get the performance of the evaluation.
    - Yes we have that, it's the exact goal. Isotopic submissions are handled this way but we haven't tried to allow which input decks.
    - Can this be expanded to include benchmarks which are the most sensitivity/energy region that is appropriate?

        - Yes, we are looking into allowing keyword to just run a type of benchmark aka 'HMF'
    - (Doro) - Will you produce the photon SCALE Libraries will you produce all the libraries?
        - Yes, link is available on the slides.

On a formal ENDF format specification language and associated interpreter

Speaker: Georg Schnabel (IAEA)

Overview: A.I. takes the ENDF-6 format and any ENDF file you have and simplifies it. In addition, this becomes an automatically formatted collection of goods (plotting, cross section blocks, formalisms used, etc). This works is using JSON to reproduce ENDF-6 formatted data. A simple exercise with MF3 was successful, however the incorporation of more complex formats (MF1) introduces new challenges. MF4 is another challenge with a mix of natural language and the list modes available to angular distributions. *Simplified* ENDF-6 manual and some developed tools available on IAEA Github.

Discussion Items:

- **QUESTION**:
    - Dave – I like this idea since this is largely how we built GNDS. Also like the idea of simplified manual and format validator, how far you along with conversion?
        - We are 90% of the way through the ENDF-6 formats. Remaining work is in MF32, MF20-28 photo atomic data.
        - Do you have access to our data repository?
            - Not sure.
        - If you get it all done, this would be really nice to integrate within the project and we'll see if the committee wants it stuffed into the manual or left adjacent but still supported by ENDF committee.
    - Nathan – What you're doing here is create an intermediate file which could be a competitor to GNDS with an ENDF structure. Would be interested in seeing with an ENDF file put into GNDS and your type to see where the strengths are.
        - Yes sounds good.
    - (Mike Herman) - I would not agree with you that this is human readable, this still has structure issues. Can add hyperlinks or references to what all of the symbols mean.
        - Further documentation on the work that has been done is required, and once this is done we can begin to talk about future-proofing and additional improvements.

SAMMY

Speaker: Dorothea Wiarda (ORNL)

Overview: SAMMY and all of its dependencies are freely available, including SCALE pieces! There will be tagging of major, minor, and beta releases. We want it given in the 'SAMMY.LPT' so we know which version to replicate/debug with. The SAMMY program flow was updated to address multiple calls to broadening/physics corrections, and has since been consolidated to handle flow control. This is to develop a rudimentary API which SAMMY can be called from to make handling and executing SAMMY easier. SAMMY modernization is primarily encompassed by moving to C++, an optimized memory

(independent C++ data class) structure for modern computing capabilities, and eliminate the enormous number of global parameters. Broadening (Doppler and Resolution) is handled through a broadening parent class which makes for faster and less redundant calls downstream. Doro has issued a formal war declaration on global parameters to streamline processing and allows for full usage of API. Documentation is moving fully to LaTeX. There is work underway to switch over to AMPX ENDF reading/writing as well as incorporate GNDS files.

Discussion Items:

- **ACTION**:
  - Eliminate all global parameters from SAMMY
  - Switch to AMPX ENDF reading and writing routines
    - Allows resources to be allocated to other improvements such as incorporation of GNDS into SAMMY
- **QUESTION**:
  - (Yaron) Will modernization of the SAMMY code allow for speed-ups for more time-consuming tasks such as doppler broadening?
    - Yes, this is in the works.
  - (Roberto) Are data sets processed and fitted sequentially? If multiple datasets are used with multiple isotopes, is the covariance produced inclusive of all correlation between isotopes and datasets?
    - (Marco) SAMMY handles everything fine, have issues exporting/recording in ENDF. Data fit sequentially, if you want one shot fit, then data must be fed together with normalization factors.
    - (Doro) Yes Marco, but GNDS can handle some of this so it is possible.
  - (Ian Thompson) We can see a future where additional correlations can be incorporated into the GNDS format, this will need to be done at some point in the future.
    - Yes, especially for reproducibility of the evaluations and uncertainty quantification.
- **RESOLVED**:
  - Significant improvements have been made to SAMMY under-the-hood to fix the problematic workflow of the code.
    - This will allow for increase modularity and robustness of the code, and support for new features.

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