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Minutes for the 2021 CSEWG Meeting

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Minutes for the 2021 CSEWG Meeting
Virtual CSEWG Meeting

15-19 November, 2021

Session chairs/document editors: D. Brown (BNL), G. P. A. Nobre (BNL), M. Chadwick (LANL), Y. Danon (RPI), T. Kawano (LANL), M. Pigni, M. Zerkle (NNL), D. Neudecker (LANL), A. Hawari (NCSU)

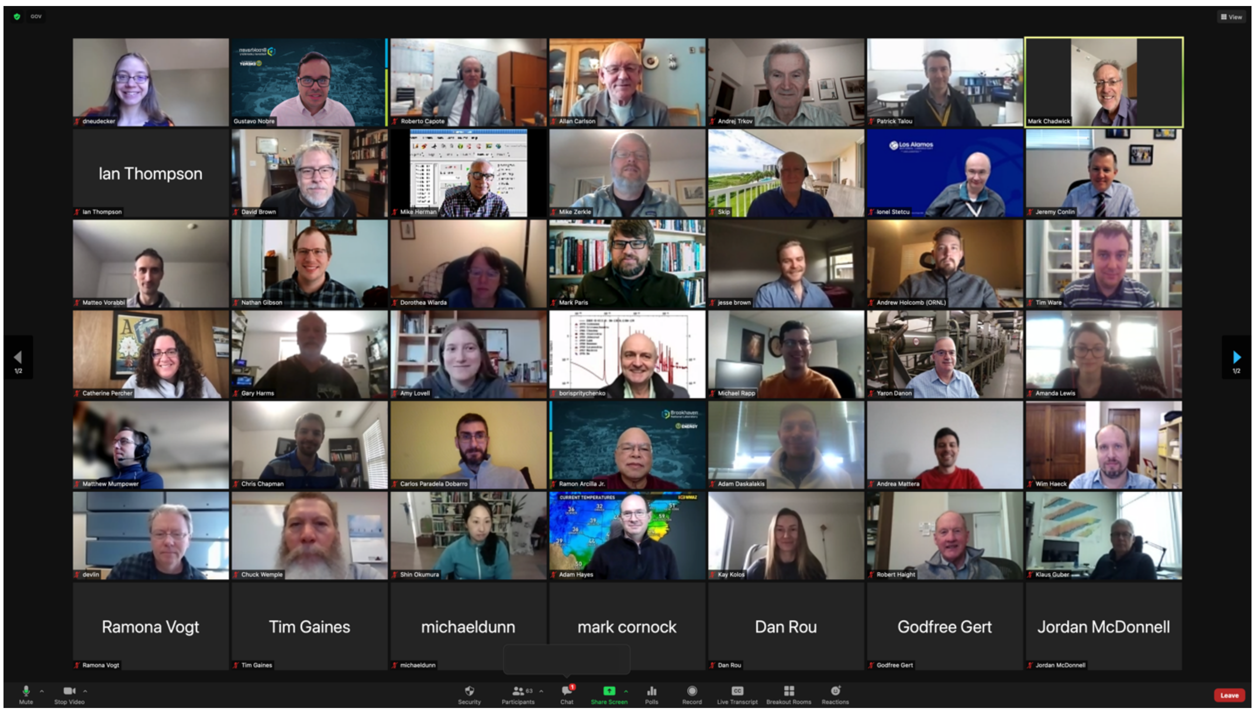

Figure 1: Zoom group photo from the CSEWG meeting.

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Introduction

This meeting is a collaboration meeting of the Cross Section Evaluation Working Group (CSEWG), a collaboration including members from various DOE NNSA and non-NNSA laboratories as well as several university groups that support these laboratory missions. The focus of this meeting will be preparations for the next major release of the ENDF/B nuclear data library. The ENDF/B library is the main neutronics library used in various US neutronics codes such as MCNP and SCALE for advance reactor work, safeguards, stockpile stewardship, etc.

This meeting served several purposes:

- Outline PuRe data implications for ENDF including metadata requirements that support DOI assignments and hence data citations.
- Use the metadata clarifications to resolve ENDF file authorship/ownership issues.
- Reestablish ENDF evaluation reviews.
- Get a status update of where we are in preparation for next ENDF release.
- Discuss whether we should "adjust" the ENDF library.
- THIS IS FROM MINI-CSEWG

This meeting was divided into 11 sessions, over 4 days, with 185 registered attendees. The first day was devoted to Formats and Covariance sessions. The second day was dedicated to Measurements and Validation. The next two days were devoted toward discussions of new evaluations for the next ENDF release. The last day was devoted to WANDA and NDAG. In these minutes, we outline the topics covered in the meeting and list any major findings or action items that resulted. The talks themselves are available at the indico meeting website (https://indico.bnl.gov/e/DATAWEEKS2021).

Monday 15 November 2021

Session: Welcome/Announcements

Time and Place: (10:00 AM-10:15 AM)
Dave Brown

At the beginning of the CSEWG meeting there were 175 Registrations for CSEWG, USNDP and NDAG combined, with about 12 Foreign nationals that could not attend because their BNL guest appointments were not approved in time. This is regrettable and we did our best to avoid it. Unfortunately, the meeting was not approved until 30 days before the planned start date, past the 35 day window requested by the BNL GUV center. Nevertheless, they did their best to accommodate us, but especially for the ones who submitted GIS late, there was not enough time to approve everyone.

There is now a new ENDF Library Manager: Gustavo Nobre. A summary of his appointments is listed below:

- 2015 to present - staff scientist, National Nuclear Data Center (NNDC), Brookhaven National Laboratory, NY.
- 2011 to 2015 - Postdoctoral research associate at the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, NY.
- 2008 to 2011 - Postdoctoral researcher at Lawrence Livermore National Laboratory, CA.
- Jun. 2007 - Ph.D. obtained on the work "Estudo do Potencial de Polarização e Fusão de Íons Pesados" (Study of the Polarization Potential and Fusion of Heavy Ions) at the Physics Institute of the Universidade de São Paulo, in São Paulo, Brazil.
- Oct. to Dec. 2005 - Internship at the University of Surrey, UK.
- Dec. 2002 - B.Sc. degree at the Physics Institute of the Universidade de São Paulo, in São Paulo, Brazil.

The CSEWG executive committee met (virtually) on October 12th and again on November 1st. Among the many topics discussed, they decided to:

- Announce new ENDF Library Manager
- Develop Code of Conduct
- Postpone ENDF/B-VIII.1 until February 2024
- Define Roles and Responsibilities of CSEWG committee (co)chairs and subcommittee chairs
- Develop agenda for PHYSOR 2021 Workshop “New physics, new capabilities, what's changing in ENDF/B”

The executive committee decided that this was needed based on past experiences. Also, attention to inclusion had never been made explicit. We thought the APS Code of Conduct was a good one to be used as a model, so a draft version of the CSEWG Code of Conduct (which was based on APS) was presented:

It is the policy of the Cross Section Evaluation Working Group (CSEWG) that all participants, including attendees, vendors, staff, volunteers, and all other stakeholders will conduct themselves in a professional manner that is welcoming to all participants and free from any form of discrimination, harassment, or retaliation. Participants will treat each other with respect and consideration to create a civil, collegial, inclusive, and professional environment at the meeting. Creating a supportive environment to enable scientific discourse is the responsibility of all participants.

Participants will avoid any inappropriate actions or statements based on individual characteristics such as age, race, ethnicity, sexual orientation, gender identity, gender expression, marital status, nationality, political affiliation, ability status, educational background, or any other characteristic protected by law. Disruptive or harassing behavior of any kind will not be tolerated. Harassment includes but is not limited to inappropriate or intimidating behavior and language, unwelcome jokes or comments, unwanted touching or attention, offensive images, photography without permission, and stalking.

Violations of this code of conduct policy should be reported to the organizers. Sanctions may range from verbal warning, to ejection from the meeting, to notifying appropriate authorities. Such disciplinary actions will be performed in accordance with the host organization's policies. Retaliation for complaints of inappropriate conduct will not be tolerated. If a participant observes inappropriate comments or actions and personal intervention seems appropriate and safe, they should be considerate of all parties before intervening.

We want to make sure we have the best minds in Nuclear Data, and we can only do that if we include all minds.

About PHYSOR 2022, it was originally conceived to advertise the release of ENDF/B-VIII.1 but considering it postponement it will be more an opportunity to show the in-progress status and an extended report. Dave Brown is organizing a ½ day workshop entitled "New physics, new capabilities, what's changing in ENDF/B". The draft agenda is:

AGENDA:

- Welcome – David Brown (BNL)
- TSL changes – supports adv. reactor and micro reactor thrusts – Ayman Hawari (NCSU)

- INDEN overview: structural materials – Gustavo Nobre (BNL) and Marco Pigni (ORNL)
- INDEN overview: actinides- Volunteers?
- Break
- FPY – Volunteers?
- GNDS-2.0 – Dave Brown (BNL) and Caleb Mattoon (LLNL)
- Summary/Discussion – Gustavo Nobre (BNL)

Session: Formats Committee

Format Tracker Issues and Proposals
Time and Place: (10:15 AM-10:45 AM)

Mike Dunn opened the Formats session stating that we will talk about Format Tracker Issues and Proposals, Processing Code Reports, Format Issues for Discussion, Status Report.

The first speaker Dave Brown combined his three talks ("Overloaded MAT numbers / misassigned MAT numbers for Al2O3 (#16)", "MAT numbers for U(UO2) and O(UO2) do not agree with ENDF Manual (#7)", and "O in BeO in UO2: MAT numbers for thermal scattering (#1)") into one.

TSL MAT number problems

There are open TSL library trackers, namely:

- #1 - O in BeO, U in UO2: MAT numbers for thermal scat.
- #7 - MAT numbers for U(UO2) and O(UO2) do not agree with ENDF manual
- #16 - Overloaded MAT numbers / misassigned MAT numbers for Al2O3

In principle these should need only a simple fix. However, we ran out of MAT numbers. The ENDF-102 manual states on page 12: "*For mixtures, compounds, alloys, and molecules (evaluations using the thermal scattering law (TSL) formats in Chapter 7), MAT numbers between 1 and 99 are assigned on a special basis (see Appendix C)*".

But the number of TSL evaluations has been steadily increasing:

- ENDF/B-VIII.0 has 33 TSL evaluations
- ENDF/B-VIII.1 already has 50 TSL evaluations
- NCrystal database has 213 evaluations

In the future we may even need more MAT numbers leading to the question of what to do?

A first option would be to stop using ENDF and cut over to GNDS. However, we are not ready to do that yet. The alternative option #2 would be to “kludge” the MAT numbers.

Kludging the MAT numbers:
Current MAT numbers use the FORTRAN I4 format:

- Option #2.1: we change to the FORTRAN A4 format and reserve 0-99 and all alphanumeric MAT designators for TSL evaluations
    - This is potentially disruptive, depending on how many legacy codes depend on MAT being an integer
    - Allows 364-900=1,678,716 TSL MAT designators
- Option #2.2: we allow TSL evaluations to use all numbers 0-9999
    - This is similar to how we handled the same issue in the decay sublibrary
    - Allows 9999 TSL MAT designators

Kludging the MAT numbers should work as MAT Numbers are used in surprisingly few places:

- End of line designators (so we can put the punchcards back in order)
- HSUB (because ENDF doesn’t have proper metadata support)
- Cross material references in covariance matrices
- As ENDF has no support for TSL covariances (unlike GNDS), we don’t need to change anything here

The (sub)options:

- Option #2.1
    - “MAT number” -> “MAT designator”
    - Chapter 1, change all ENDF formats to use the FORTRAN A4 format, plus associated discussion
    - Update the HSUB format (it is free text already)
    - Update the TSL example
    - Add note in the covariance chapters about not changing MAT numbers here
    - Appendix A summary table
    - Appendix C now can be made to work
- Option #2.2
    - “MAT number” -> “MAT designator”
    - Chapter 1 update rules
    - Appendix C now can be made to work

It was noted that Option #2.2 causes the least disruption as had been pointed out by Wim Haeck in an earlier discussion. This is also a problem for the decay sublibrary.

This change has already been implemented as Merge request #10 “A better MAT number rule”. The Appendix C has not been changed yet, as it is better to wait until we know full scope of the TSL changes.

During the time allocated for questions, somebody pointed out that it is needed to have a table with the MAT numbers to avoid inconsistencies. As answer, Dave said that we still need to search for duplicates. Instructions are more guidelines than rules, and some need to be rethought.
Additional comments from the community:

- TENDL does not have MAT numbers because there are so many materials
- This should allow for thousands of new MAT numbers, which should be enough until we can totally switch to GNDS.
- Why worry about a rule if we will have a crib sheet mapping the MAT number to the materials?
- Crib sheet is to avoid confusion with new TSL evaluations.
- Comment: Can include new MAT numbers in TSL evaluation comments

This is a format change proposal. It was voted and moved to approve, as nobody was against it.

Mike Dunn/Andrej Trkov: described issue #106 about the Temperature specification in the ENDF file. If you have resonance parameters, the temperature in file 1 should be zero. In case of iron for example you have fluctuations in the fast range, but if you want to do Doppler broaden it you have to be able to see it at zero temperature, reconstruct cross sections, and then Doppler-broaden to the desired temperature. You should have zero temperature when there are resonance parameters.

Doro pointed out that one paragraph in the format proposal is confusing. Andrej argues that it is clear because if fluctuations go above resonance range, it should be Doppler-broadened up to higher energy (assumed to be room temperature) beyond the resonance range. In the end, what Andrej proposes is a clarification in the manual, as it shouldn't impact any previous evaluation.

Mark Paris asked if the text in the issue tracker is the actual text proposed as recommended change to the manual. Indeed, the last few paragraphs of the tracker is the proposed change. Dave said that we need an actual merge request with the actual text.

Action items: Andrej needs to submit a merge request with the proposed text change.

NJOY - LANL
10:45 - 11:05
Wim Haeck

Just a little NJOY update

Agenda:

1. 1.Getting NJOY2016 ready for ENDF/B-VIII.1
   a. Overview of features to be supported
   b. ACE format changes
   c. NJOY2016.66
2. Modernisation updates
   a. ENDFtk
   b. ACEtk
   c. GNDStk

Making a new ENDF/B library …

- Every new ENDF/B generation changes formats and adds new data
- The future library: ENDF/B-VIII.1 (somewhere in 2024)
  - Mixed mode thermal scattering (coherent and incoherent elastic scattering)
  - Background R-matrix elements for resonance parameters in MF2 MT151
  - Improved photonuclear data
- If these changes impact the ACE format, MCNP needs to be updated too
  - These changes are prioritised due to the involvement of MCNP
  - Changes are made in collaboration with the MCNP development team
- MCNP6.3 will have experimental support for these new ENDF/B-VIII.1 features

Thermal scattering:

- Nuclear data evaluations identify multiple categories of thermal scattering:
  - Coherent elastic: important in crystalline solids (graphite, metals, etc)
  - Incoherent elastic: important in solids with hydrogen (polyethylene, ZrH, etc.)
  - Coherent and incoherent inelastic: all solid and liquid materials (hydrogen in water)
- Prior to ENDF/B-VIII.1: either coherent or incoherent elastic scattering
  - Coherent and incoherent are not exclusive and neglecting one is an approximation
  - ENDF/B-VIII.1 will introduce mixed mode elastic scattering
- This feature is reflected in the ACE format itself
  - Only one elastic thermal scattering data block, which is either coherent or incoherent
  - We needed to add an optional second block when both are given

The original thermal scattering format in ACE:

- The thermal scattering format is relatively simple:
  - Two main blocks: one for inelastic and one for elastic
  - The elastic block is either coherent (IDPNC=4) or incoherent (IDPNC=3)
  - Formatting parameters given in the NXS array
- The old format is still VALID:
  - When mixed mode is used, there will be an additional elastic block (IDPNC=5)

- Coherent elastic is always given first, incoherent elastic is given after that
- An additional formatting parameter: NCLI for the second elastic block only
    - NCL will always be -1 for IDPNC=5 (for both coherent and incoherent)

A few examples were given:

- Example: H-H2O - inelastic only H IN H2O @400K FROM ENDF/B-VIII.0 - CHECK TAPE 1 Thermal cross sections: Showing that we produce the same results.
- Example: Al27 metal – coherent elastic and inelastic AL-27 @400K FROM ENDF/B-VIII.0 - CHECK TAPE 1 Thermal cross sections
- Example: Zr-ZrH – incoherent elastic and inelastic ZR IN ZRH @400K FROM ENDF/B-VIII.0 - CHECK TAPE 1 Thermal cross sections
- Example: D-7LiD – mixed mode elastic and inelastic D IN 7LID @400K FROM ENDF/B-VIII.1-BETA - CHECK TAPE 1 Thermal cross sections: New style of evaluation with both coherent and incoherent modes.

Photonuclear data:

- Traditional photonuclear data
    - Secondary photon distributions traditionally given using the LAW=1 LANG=1 format
    - Traditionally using a single Legendre coefficient (i.e. isotropic distribution)
    - This assumption was hardcoded in NJOY2016's ACER module
- And then the IAEA-2019 library was released (August 2020)
    - Secondary distributions are using anisotropic Legendre expansion
- NJOY2016 had to be updated
    - A temporary fix was introduced to keep the distributions isotropic
    - A permanent fix now translates the distributions properly into ACE LAW=61
    - Only MCNP6.3 is capable of using these new photonuclear files

Example:

- Mono-energetic photon beam on a ^{239}Pu disk
    - Neutron spectrum tallied outside the disk in a 0.1 mm sphere
        - Using ENDF/B-VIII.0 photonuclear data
    - Comparing ENDF/B-VIII.0 with IAEA-2019
        - Only MCNP6.3 can run the IAEA-2019 ACE files

New evaluation reproduces VIII.0 fission spectra

NJOY2016.66

- This is a big update, the major changes are:
    - The photonuclear data format changes (ACE LAW 44 to 61)
    - Mixed mode elastic scattering in thermal scattering laws
- ACER

    - Photonuclear ACE format update (including plots and output file)
    - Formatting/processing the thermal scattering data (including plots and output file)
    - The XSS array and its size is now set in the common acecm module
    - Added locator checking and unknown law checking when writing out ACE files (When this happens, there is an issue that can cause MCNP problems. These things previously went undetected)
        - NJOY2016 will now error out when locators are inconsistent or when an unknown law is used § Previously only for incident neutron and charged particle CE files
        - Extended to photonuclear and thermal scattering files
    - Some changes in the input file for mixed mode elastic (card 9: ielas=2)
    - Charged particle updates
- MODER
    - MF7 and MF28 update
- THERMR
    - Most of the thermal scattering processing happens here
    - Between 1 and 3 thermal scattering MT numbers are added to the PENDF file
- ERROR
    - Fixed a crash caused by MF34 covariances using multiple subsections
    - Each subsection is now processed but we are still working on outputting the results
- Additional non-regression tests
    - There are now 71 cases in the NJOY2016 test suite
    - Tests 67-70 provide tests for all combinations of thermal scattering data

What does the future bring?

- NJOY2016 will be maintained for the foreseeable future
    - NJOY2016 is essentially the production code at LANL
    - New formats for ENDF/B-VIII.1 will be supported:
        - Thermal scattering: mixed coherent and incoherent elastic scattering
        - External R-matrix elements used in some new resonance evaluations
- NJOY21: shift from a module based to a component based modernization
    - Modernised modules are built from components
        - Components provide formats (ENDF, ACE) or processing operations (resonance reconstruction)
        - Components can be developed and deployed faster than modules
        - Components provide features that modules do not provide
    - Using a C++ and Python API at the same time

Processing components are format agnostic:

- In the beginning there was only ENDF …
  - As a result, NJOY2016 is very closely linked to ENDF
  - Introducing the new GNDS format in NJOY2016 is practically impossible
- NJOY21 processing components MUST be format agnostic
  - Internal data structures that reflect generic data can be built from scratch
  - Build these data structures using ENDF or GNDS evaluated data, or other user data

NJOY21 formatting components:

• ENDFtk - Evaluated nuclear data format (the legacy one): almost everything in the ENDF format, including internal NJOY sections:

– Some of the covariance sections are still missing
– GENDF support (for GROUPR and ERRORR) will be added soon
– https://github.com/njoy/ENDFtk

• ACEtk (Application library format for MCNP) and GNDStk (Evaluated nuclear data format (the new one)) will be our focus for FY22:

– https://github.com/njoy/ACEtk
– https://github.com/njoy/GNDStk

Current status of ACEtk

Hopes to finish this by the end of calendar year

Current status of GNDStk:

- The GNDStk development approach
  - A tree/node based core interface that is GNDS standard agnostic
  - A GNDS standard interface layer
    - An autogenerated interface that follows the GNDS standard specifications
    - Both a C++ and python interface is generated
    - Allowing for customization to produce a slimmed down and abstracted interface
- GNDStk v0.1.0 is a prototype using a slimmed down GNDS 1.9 standard
- We're in the process of implementing the GNDS 2.0 standard
  - The autogenerated interface should be ready by now (at least I hope it is)
  - Customisation will begin for resonance parameters and cross section data

A first application: plotting

Conclusions:

- NJOY2016 will be maintained for the foreseeable future
  - New formats for ENDF/B-VIII.1 will be supported
  - NJOY2016.66 already implements a few of these
  - Experimental support for the ACE format changes in MCNP6.3
- NJOY21 modernisation
  - Component based versus module based
  - C++ and python interfaces
  - Currently focus is on format components: ENDFtk, ACEtk, GNDStk

After the talk there were some discussions:
Q: Can these toolkits be used to modify data and write back to ENDF?
A: @Devin Yes, that's one of our use cases. Supporting evaluations, perturbations, etc., is a nice added benefit of these.
Some of the details of that are worth another discussion.

AMPX and SAMMY Status Report
Andrew Holcomb and Doro Wiarda
11:05 - 11:25

PUFF/COGNAC Improvements

- If it is a minor roundoff problem, we bump the values back into the valid range, and report it (as in SCALE6.2)
- If an egregious error (outside of precision) is detected for ANY matrix element, PUFF and COGNAC (AMPX covariance modules) will now:
  - Set self correlation matrices to the identity matrix
  - Set cross correlation matrices to the zero matrix
- In practice, this has only affected a small subset of isotopes in the ENDF-8 covariance library

SCALE 6.3 Data

- ENDF-7.1
  - Corrected probability tables for subset of evaluations (in MG & CE)
  - New coupled MG libraries, xn252g47v7.1 and xn56g19v7.1
    - gamma group structures identical to v7.1-200n47g and v7.1-28n19g
    - neutron group structures identical to v7-1.252 and v7.1-56
  - New Sodium Fast Reactor (SFR) MG library, 302 groups
  - New general-purpose MG library, 1597 groups

- ENDF-8.0
  - MG libraries
    - Distributed in 252 (thermal), 302 (SFR), and 1597 (generic) groups
    - Shielding libraries in 200n47g and 28n19g format
  - CE library now distributed in HDF5 format
  - Covariance data in 56 groups (includes best estimate augmentation)
  - 56 group perturbation libraries for SAMPLER

- Removed all ENDF-7.0 libraries (kept all ENDF-7.1 libraries)
- Standard composition library is now rev40 (rev38 and rev39 removed)
- Removed ORIGEN JEFF activation libraries with no corresponding transport library structure (44, 47, 49, 238)
- Removed obsolete helper data no longer required by modern sequences

Note: SCALE 6.2 data is still fully operational with SCALE 6.3. A limited set of SCALE 6.3 data can be used with the 6.2.* series.

Thermal Scattering Law

- Short Collision Time subroutine and angular gridding improvements currently under review for inclusion in future AMPX release
- Implementation of mixed elastic scatting format underway
  - Combining incoherent elastic & inelastic into same MT number to save space
  - Will be backwards compatible for all TSL files with incoherent elastic & inelastic data

How to Support GNDS:

- Internal AMPX C++ structures are the "API" that AMPX and SAMMY will access.
- Add a Reader/Writer that supports GNDS and fills AMPX internal C++ structures.
- Test by processing ENDF formatted and GNDS formatted files and compare results.
- Find an efficient way to support GNDS which also allows us to easily apply updates.
- Updates might not immediately be propagated to the internal AMPX C++ classes if not needed in AMPX.

GNDS access layers in AMPX

- Python generated C++ classes for all objects described in the GNDS specification. Generation is based on the JSON files of the GNDS standard. Approx. 290 classes are generated. All inherit from GNDElement.
- Special names are selected for GNDS objects such as Double, which have names not allowed in C++.
- Namespaces are handled as in the GNDS specification, thus the same name but in different namespaces is allowed.
- Some correction for errors in the specification are built into the Python generation code. If corrections are applied, they are reported.

These classes are a very low-level access API to the GNDS content, that mirror the specification directly.

Classes that fill the AMPX C++ in-memory structures. These classes are needed as:

- To select the correct “style” of the data the user requested, which includes following the inheritance chain.
- Convert GNDS units to AMPX units
- Convert GNDS constructs into AMPX constructs.
- More user-friendly access methods to Particle data base

This layer is currently only reading data, but writing will be added as needed. The first implementation for reading will be for resonance parameters and corresponding covariance matrices for use in SAMMY.
These classes are available in the SCALE 6.3 release.

- Python code for generating low-level C++ routines as well as the generated files are available open source: https://code.ornl.gov/RNSD/gnds.
- Currently works for GNDS-1.9, (a small fix is needed for the master branch – patch available in the repository).
- C++ classes support reading and writing.
- We are in the process of updating to the upcoming GNDS-2.0 specification.

SAMMY/AMPX and GNDS – future plans:

- SAMMY has its own ENDF reading and writing routines.
- We plan on switching to the AMPX reading and writing routines. This was delayed in favor of using in-memory C++ AMPX classes for resonance parameter and all covariance information.
- Having the relevant information in the in-memory classes will make it much easier to switch out the reading and writing to use AMPX methods.
- AMPX is in the final stages to add support for reading GNDS formatted ENDF files.
- Switching to these routines will bring GNDS support to SAMMY. In this context, writing of GNDS files will also be added.

SAMMY overview:

- Updates in the covariance matrix storage and access which allowed more robust handling of radius parameters and pup'ed parameters
- Derivatives and cross sections are now stored in a C++ grid
- New framework for the 0K resolved resonance reconstruction.
- Preliminary API for use with alternative fitting routines

Covariance storage:

- All covariance information is stored in the same C++ object used in AMPX. Including:
    - Resonance parameter covariances (including pup'ed parameters)
    - Data covariance

    - Implicit data covariance information
- This allows the removal of various scratch files.
- Created a helper C++ class that keeps track:
    - Were adjusted parameters are stored in the covariance matrix (decoupling the input order and calculation order)
    - Whether a parameter is a pup'ed parameter

This helps especially for parameters that are coupled, for example all radii are the same or all gamma width for a given spin group (several bugs related to this were found and corrected). In the future this will allow more user-friendly output formats for covariance information.

Updated Derivative Classes:

- Last year we reported that we added a C++ class for the final cross section and derivatives.
- We added a derived class that keeps track of cross section and derivatives throughout SAMMY:
    - The class manages zero suppression for derivatives that can only be non-zero for a given isotope Needed if the sample contains more than one isotope, where the cross sections and derivatives will be collapsed to the sample cross section before the adjustment
- The use of the class again allowed the removal of several scratch files.
- Internally SAMMY has two types of adjusted parameters:
    - Only non-zero for a given isotope (like resonance parameters)
    - Potentially non-zero for all isotopes (like normalization parameters)
- While the new class allows to remove those two types of parameters (as it handles the needed zerosuppression) it is currently only used in the resolved resonance reconstruction.
- With the use of the new class, the order of the parameters (needed to distinguish between the two) will no longer matter. This will make it much easier to add additional parameters.

Frame-work for 0K resolved resonance range:

SAMMY support several different resonance formats in the resolved range. In addition, we would like to connect the AMPX version to this mix.

- For each of these formalism there was a lot of duplicate code related to the looping over the energies, transformation to transmission if desired, etc.
- All formalism depend on SAMMY global parameters, which makes code re-use hard.
- We created (still in Fortran):
    - CrossSectionCalculator, containing information common to all formalism (like resonance parameter and covariance information) plus a function to calculate the cross section and derivatives for one energy. Child classes for all supported RR formalisms exist.
    - CrossSectionCalcDriver, a class that selects the correct class of CrossSectionCalculator

- ZeroKCrossCorrections, a class that calculates the 0K cross section and derivatives on all energies and applies desired 0K corrections.
- We reused the existing Fortran code for all the formalism but references to SAMMY global parameters have been mostly removed.
- We plan to connect our existing AMPX resonance API to this framework.

Preliminary API:
The program flow in SAMMY is not very yet structured so that we can easily add an API to allow for access to SAMMY from external programs. However, it would be advantageous to use SAMMY to calculate cross section data and derivates including experimental corrections to evaluate for example different fitting algorithms. In order to investigate this, we have added a very preliminary API that:

- Reads the usual SAMMY input
- Stops right before an adjustment step, i.e. after calculating the cross section and derivatives.

This API is currently used for in the Monte Carlo evaluation project in conjunction the Metropolis-Hastings algorithm

Discussion:

Q Devin Barry: Will AMPX will be open source?
A: Yes. Main focus has been to put SCALE 6.3 out the door. Will then reorganize SCALE so we can separate parts that are Export Control and what is non-EC can be made available in git repo.

Q Denise Neudecker: Are issues with covariance in issue tracker?
A: Wasn't aware there was an issue tracker, but can make issues available
Q: Are those issues fixes
A: Believe so, will make sure they are.

FUDGE - LLNL
11:25 - 11:45
Bret Beck

FUDGE: LLNL nuclear data infrastructure

Overview of FUDGE

- For Updating Data and Generating Evaluations (FUDGE)
- Use to read/write, plot, modify and process GNDS data

    - Processing for Monte Carlo and multi-group transport.
- User interface is python 3.6+.
    - Computationally intensive stuff written in C and C++.
        - E.g., heating cross sections, multi-grouping distributions.
        - Users do not interact directly with the C and C++ codes, the python interface handles that.
- FUDGE is like a toolkit but we are writing many scripts that are included in the bin directory
- FUDGE can convert ENDF-6 (and LLNL ENDL) files into GNDS, and GNDS to ENDF-6.

FUDGE processing example for transport codes

- FUDGE command to process a GNDS file for deterministic and Monte Carlo transport at 3 temperatures (MeV/k)

```
bin/processProtare.py -mc -mg -t 2.58522e-08 -t 1e-07 -t 1e-4
gnds.file.xml
```

- Output (i.e., processed) file contains
    - evaluation data
    - Reconstructed cross sections (if needed)
    - Coulomb + nuclear elastic μ cutoff (if needed)
    - average product data (needed for energy deposition - KERMA)
    - pdf/cdf data for distributions (e.g., P(E'|E))
    - heated cross sections (at 3 temperatures in example above)
    - Common grid heated cross section for Monte Carlo (ditto)
    - multi-group data (ditto)
    - TNSL data, if present, are processed FUDGE processing example for transport codes

URR processing is done separately, still needs to be integrate in.

GNDS 2.0 support in FUDGE:

- GNDS 2.0 has not been officially released but it is most likely complete except for a few minor requests.
- FUDGE is up-to-date to handle GNDS 2.0
    - Except for TNSL (see Caleb) and that's because the specification are still being tweaked.
- Internally, FUDGE looks a lot like GNDS 2.0
    - I will show examples later
- Since GNDS 2.0 is not finalized, FUDGE writes the format as '2.0.LLNL_4'.
    - We have generated '2.0.LLNL_4' file for ENDF/B-VIII.0 that the OECD/NEA will make available (see Michael Fleming)

FUDGE creates many "nodes" automatically.

- For example, in GNDS 2.0 the top node “reactionSuite” has the following child nodes:
    - externalFiles
    - styles
    - PoPs
    - resonances
    - reactions
    - orphanProducts
    - sums
    - productions
    - incompleteReactions
    - fissionComponents
    - applicationData
- All of these are automatically created by the “reactionSuite” constructor (i.e., “__init__”) except for the “resonances” node and I will try to fix that.
- All child nodes but “PoPs”, “resonances”, “sums” and “resonances” have an ”add” method to add an object.
- Adding an instance to reactions example
    - reactionSuite.reactions.add(reaction)

GNDS 2.0 documentation node support in FUDGE

- The documentation node in GNDS 2.0 allows one to record a lot of information (thanks mainly to Dave Brown).
- Child nodes are:
    - authors, contributors, collaborations, dates, copyright, acknowledgements, keywords, relatedItems, title, abstract, body, computerCodes, experimentalDataSets, bibliography and endfCompatible.
- All child nodes are automatically created by the documentation constructor
- Next slide show how to populate *title* and *abstract* nodes.

Documentation example

Note, only nodes that have been populated are written to a file.

GNDS 2.0 map file supported in FUDGE and GIDI+

A map file supports nesting which is used by EMU.

LLNL also has multi-group boundaries and flux files

- Multi-group boundaries format uses GNDS `<group>` node to store the label and boundaries for a group.
- Flux stored as f(T,E,mu) using a GNDS 3d function.

Plotting example for ‘n + U230’ via pyQt5 and matplotlib

Plot is interactive

Check for missing gamma data in ENDF-VIII.0

This example ignores nesting of products, but the code I used did include nesting.

FUDGE scripts

- We are developing scripts to make it easier to examine and process GNDS files.
- Some examples include:
    - processProtare.py: Processes for Monte Carlo and multi-group transport
    - peek.py: Prints each reaction and brief information about each reaction's products.
    - temperatures.py: List all temperature data in a GNDS file
    - checkGNDS.py: Check the physics in a GNDS file (e.g., positive cross sections, normalize distributions)
    - diffGNDS.py: Does a partial diff of two GNDS files
    - buildMapFile.py: Creates a map file from a list of GNDS files
    - checkMap.py: Check a map file and all it reference

Some of what are we working on in FUDGE

- Improving URR probability table building
    - We are working to BNL on this (Dave Brown and Matteo Vorabbi)
    - Currently, not automatic in FUDGE
- Adding a multi-group sums node to reduce load time for deterministic transport codes
        - Initially, this will go under the “applicationData” node
    - § Additional ACE support

      — Currently supports GNDS to ACE for neutrons transport including TNSL
    - § Update codes for GPUs where possible and beneficial (e.g., heating cross sections, calculating multi-group transfer matrices)

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FUDGE refactoring

- We have been doing some needed refactoring of FUDGE
- Latest release includes most of the refactoring but still have more to do
- Hope to complete refactoring by January 2022 and do another release
- That said, anyone interested in FUDGE should get the latest release and play with it since a few small changes should be needed to update scripts for the January release

Other talks related to FUDGE:

- Caleb Mattoon will be talking on TNSL data and FUDGE
    - Talk Wednesday at 10:00 am EST
    - "TNSL Implementation and Testing in FUDGE"
- Kyle Wendt will be talking on EMU
    - Talk today at 17:35 EST
    - "An Uncertainty Quantification Toolkit for GNDS Formatted Libraries"
    - Evaluated Means and Uncertainties (EMU)
    - Generates realizations from mean and covariance data
    - Uses FUDGE to read/write and modify data.
    - Also generates processed files

GIDI+:

- A collection of packages for transport codes to read GNDS files
    - Mainly written in C++
- GIDI+ consists of the following packages:
    - PoPI: Property of Particles Interface
        - Reads PoPs data
    - GIDI: General Interaction Data Interface
        - Read in a GNDS reactionSuite file
        - Supports map files
        - Includes support for multi-group data including collapsing
        - Currently, only reads GNDS data needed by transport codes
    - MCGIDI: Monte Carlo GIDI
        - For use in Monte Carlo transport codes
        - Extracts needed data from a GIDI instance
        - Has cross section, energy deposition, etc. lookup functions by temperature and energy
        - Has reaction, distribution sampling functions.
    - plus other packages rarely called directly by transport codes

What are we working on in GIDI+:

- Decreasing load times
    - 'lazy reading'
    - Summed data for deterministic transport codes

- Direct sampling of elastic TNSL data
    - from S(E,T) for coherent elastic
    - from DebyeWaller - W'(T) – for incoherent elastic
- Updating the version in GEANT4
    - Current version is many years old and does not read GNDS
    - We have funding to work on improving diagnostic gammas
        - Dave Brown and BNL leading effort
- Add physical unit support
    - Already in FUDGE

Code releases

- We are releasing all codes under https://github.com/LLNL
    - FUDGE
        - https://github.com/LLNL/fudge
        - Version 5.0
        - Python 3.6+
        - Pip install – instructions on github site
        - BSD license (will switch to MIT license)
        - GNDS format is 2.0.LLNL_4 which should be the same as 2.0 if there are no further changes to GNDS 2.0 specifications (except for TNSL data)
    - GIDI+
        - https://github.com/LLNL/gidiplus
        - Version 3.22.??
        - C++11
        - GNDS format is 2.0.LLNL_4 (and 2.0?)
- Releasing all codes under MIT license, except currently FUDGE

Final comment

- Latest releases of FUDGE and GIDI+ will be available in a few days.
- Plan to do another release around 1 Jan. 2022.
- If you find any issues with FUDGE or GIDI+ please let us know
- We plan to also release EMU (see Kyle Wendt)
- We need you to look at the latest 2.0* including
    - The specification document
    - the NEA files
    - What FUDGE is doing (i.e., it is doing something wrong)

Inconsistent use of the characteristic bound cross section for incoherent elastic scattering (#13)
12:40 - 12:55
Jose Ignacio Marquez Damian (European Spallation Source)

The order of the talks was switched and Damian decided to present first with the actual talk title “Free atom scattering cross sections and normalization of thermal scattering data.”

Acknowledgments:

- To Danila Roubtsov, with whom we started discussing this for the normalization of the thermal scattering evaluations in JEFF 3.3 and ENDF/B-VIII.0
- To my colleagues at the European Spallation Source, particularly Thomas Kittelman, who brought back this discussion for the normalization of data in NCrystal: Cai, X-X., and Thomas Kittelmann. “NCrystal: A library for thermal neutron transport.” Computer Physics Communications, 246, 106851 (2020).

Neutron and thermal scattering sublibraries:

- Neutron sublibrary
  - Information is given per nuclide
  - Nuclear interaction is complex
  - Condensed matter physics is simple
  - Angular momentum is important
- Thermal scattering sublibrary
  - Information is given per compound.
  - Nuclear interaction is simple (constant scattering lengths or cross sections)
  - Condensed matter physics is complex
  - Neutron spin and coherence is important

Example of different elastic cross section

More complexity:

- In thermal scattering, neutron wavelengths are similar to the interatomic distances, producing interference effects.
- These interference elastic and inelastic effects are proportional to the bound coherent cross section.
- The remainder is the bound incoherent cross section.

Example of scattering where both coherent and incoherent contributions are important

Compilations and sources:

- Sears, V. F. ”Neutron scattering lengths and cross sections.” Neutron news 3, no. 3 (1992): 26-37. Available online: https://www.ncnr.nist.gov/resources/n-lengths/list.html
- Koester, L., H. Rauch, and E. Seymann. ”Neutron scattering lengths: a survey of experimental data and methods.” Atomic data and nuclear data tables 49, no. 1 (1991): 65-120.
- Dawidowski, J. et al. ”Neutron scattering lengths and cross sections.” In Experimental Methods in the Physical Sciences, vol. 44, pp. 471-528. Academic Press, 2013.
- Experimental data is also available in EXFOR (BA,AMP; BA,SIG; FA/INC,SIG; FA/COH,SIG).

(but these sources are not necessarily consistent with evaluated nuclear data libraries)

Some examples

- NCrystal (based on the data from Koester): https://github.com/mctools/ncrystal/blob/master/ncrystal_core/src/NCAtomDB.cc
- JEFF 3.3, reconstructed at T=0K with NJOY into ACE and plotted with OpenMC.
- ENDF/B-VIII.0, reconstructed at T=0K with NJOY into ACE and plotted with OpenMC.

Some examples were given, where:

- The difference is small
- Asymptotic value is still close.
- Doesn't go asymptotically to the straight line.
- Big discrepancy
- Big discrepancy again, but now the bigger cross section is switched.

Other examples of discrepancies were given (Ca…)

Conclusions

- Thermal scattering evaluations require values for normalization, which should be compatible with evaluations in the neutron sublibrary.
- One normalization, σfree, can be extracted from the asymptotic value of σel(E , T = 0K), but we need also to separate it into σinc, σcoh.
- Reconstruction at T = 0K is a simple test that can be automated and incorporated into V & V pipelines.
- Artifacts and inconsistencies are easy to spot.

Questions / challenges:

- Can we obtain b −, b + from the nuclear evaluation codes and store them in MF=1 / MT=451?
- Scattering lengths and cross sections can be measured with great precision using thermal scattering techniques. Is this feedback useful for nuclear evaluations?
- These questions were always there, but latent, because thermal scattering libraries were limited to a few materials. But new tools, like NCrystal, are changing the scenario: https://github.com/mctools/ncrystal/wiki/Data-library

TSL Issue # 13 Inconsistent use of the characteristic bound cross section for incoherent elastic scattering:
https://git.nndc.bnl.gov/endf/library/thermal_scatt/-/issues/13

- The normalization value for the incoherent inelastic reaction (MF=7/MF=4) is stored as $M_0 f_0$, the product of the numbers of atoms times the free atom cross section.

- The normalization value for the incoherent elastic reaction (MF=7/MF=2) is stored as σ_b^{inc} , without multiplying by the numbers of atoms.
- THERMR divides both by M_0, but AMPX does not.
- The evaluation for H(CH2) historically follows the NJOY convention.

TSL Issue # 13 Possible solutions:

- Change the field in the ENDF-6 format to be Mn*σ_b^{inc} , or
- Change NJOY to divide the free atom cross section by Mn, but not the bound elastic cross section. Also, fix polyethylene, lucite and revert the change in solid methane.

Comment from Doro: We should change the manual to take from the S(alpha,beta). To which José Ignacio agreed.

Mike Zerkle suggested to revise NJOY. José points out then that one would need to change lucite, polyethylene and other evaluations. Wim says the best solution is to have NJOY doing it properly. Wim suggested providing a warning in case someone is using an outdated evaluation.

Action Doro and Chris should sort out the process and see what the recommendation should be and work with Ignacio and Wim.

Isotope Effects in Thermal Neutron Scattering
12:30 - 12:40
Andrew HOLCOMB (Oak Ridge National Laboratory)
WIARDA, Dorothea (ORNL)

Background

- AMPX links Thermal Scattering Law (TSL) libraries to isotopes in the resolved resonance region
    - TSL eval explicitly names isotope, we only bind TSL data to that isotope
        - tsl-013_Al_027, tsl-026_Fe_05
    - Otherwise, assumes all isotopes can apply the TSL eval
        - tsl-reactor-graphite-10P -> ^{12}C-10p-graphite, ^{13}C-10p-graphite
        - U-UO_2 -> $^{233}UO_2$ + $^{234}UO_2$ + $^{235}UO_2$ + …
        - Zr-ZrH -> ^{90}ZrH + ^{91}ZrH + ^{92}ZrH + …
- No guidance is given in the TSL files or the ENDF format if this is acceptable or advised
- This can lead to some issues…

Different Scattering Lengths

- Isotopes of the same element can have significantly different scattering lengths and, therefore, different bound/free scattering cross sections

- Element-specific bound/free scattering cross section given in File 7, but not sub-divided into isotopic distribution
- User must rely on either description in the ENDF file or references, which may not provide necessary description
- Different from issue in incoherent elastic bound scattering cross section issue (#13)

Different Scattering Lengths – Comparison of Elemental and Isotopic Free Scattering Cross Sections

- Examples of comparisons of elemental and isotopic free scattering cross sections for Zr and Si were given, taken from Ref [1].
- Up to 50% difference between isotopic & elemental scattering cross sections can be observed

Plots were presented showing the discrepancies of scattering lengths between elastic cross sections of ^{90,91}ZrH and ^{90,91}Zr.

Resonances

- Some isotopes have resonances near (or sometimes IN) the thermal range
- Resonance theory is not currently incorporated into thermal scattering evaluations
- These can have a noticeable effect on the thermal scattering cross section

Currently these effects of resonances in/near thermal region have been ignored.

Discussion

- Should information about the isotopic composition be provided in ENDF TSL files?
- Can anything be done regarding low-lying resonances?
    - Try and match the TSL cross section with the resonance at a specific cutoff energy (tricky, but doable)?
    - Implement resonances in thermal scattering (very difficult)?

Comment from Mike Zerkle: There is a need for bound scattering and scattering cross sections evaluations for low-A materials

Comment from Ayman Hawari: The discussion should focus on how transition from TSL to the neutron cross section.

References:

[1] https://www.ncnr.nist.gov/resources/n-lengths/

Unresolved Resonance Region
13:10 - 13:40
Andrew Holcomb, Dorothea Wiarda.

Introduction

- The ENDF format in the URR has several limitations
- Some of these limitations are addressed in GND

The following slides are **not** aiming to present a solution.
We would like to briefly outline the limitations and foster a discussion that can lead to format proposals.

URR format for resonance parameters

- SLBW only
- Average resonance parameters are given at one or more energy of reference
- Covariance can only be given at one energy of reference, .i.e. on resonance parameters averaged over the whole region.
- Conflicting advice in the manual concerning the interpolation between energies of reference

Resonance formalism

- SLBW only:
    - Advantage:
        - Temperature and background dependent cross section can be calculated analytically at a given energy
        - The formalism might be good enough given the cross section in the URR
    - Disavantage:
        - Energetically allowed channels (for example discrete inelastic, MT=51 and others) cannot be included in the URR. Can be included as point-wise data but are then excluded from self-shielding calculations via probability tables.

GND explicitly gives the algorithm, only SLBW is currently allowed.

Competitive width

- For evaluations where we know that the evaluator intended it:
    - AMPX can interpret the competitive width as the width for MT=51
- Our codes have input flags that switch this behavior on or off, with off being the default.

Covariance data in the URR
The restriction might lead to a disconnect between parameters and covariance and makes it harder for evaluation codes like SAMMY to generate the covariance. Processing codes like AMPX can generate the desired group averages. GND also gives the covariance on average parameters, but it allows to give the energy range to which they apply. In principle different covariance information can be given for each range to which an energy of reference applies.

Interpolation in the URR

- Some codes (AMPX) take the first part of the recommended procedure and omit the second part
- AMPX can switch to interpolation on parameters provided that the user defines the energies at which parameters are to be interpreted to in the input.
- It might be advantageous to add a flag in the format that allows to specify the desired interpolation. Such a flag would lead to more consistent behavior across processing codes.

Question from Andrej Trkov: Can SAMMY calculate uncertainties in the cross section domain? You can put the covariances into MF=33. If so, that's probably the better solution. Doro agrees. It solves the issue if the mesh is dense enough in URR would be dense enough that the cross section can be linearly interpolated. Doro agreed but warned that the manual needs to be updated.

Dave Brown reminded that unresolved resonances are expected to fluctuate. URR should be treated in terms of the probability tables. He pointed out that Matteo Vorabbi will present something related to this in the covariance session.

Roberto Capote: Sometimes we know the position of some of the resonances.

CSEWG: Formats Committee - Status Report
13:45 - 14:30

Status of EG-GNDS
Dave Brown

GNDS-1.9 specifications published Summer 2020

- Specifications: https://oecd-nea.org/download/wpec/documents/7519-GNDS.pdf
- XML Schema for GNDS-1.9: https://www.oecdnea.org/download/wpec/gnds/gnds.xsd
- GNDS Webinar: https://www.youtube.com/watch?v=h9Byrkxr8LE&feature=youtu.be

Thank you webinar participants
https://www.youtube.com/watch?v=h9Byrkxr8LE&feature=youtu.be
The NEA hosted an expert roundtable webinar on GNDS on 8 July 2020. The discussion was be moderated by William D. Magwood, IV, NEA DirectorGeneral and Dr David Brown (BNL), Chair of the NEA Expert Group on the Recommended Definition of a General Nuclear Database Structure (GNDS). The panellists included:

- Dr Osamu Iwamoto (JAEA)
- Dr JeanChristophe Sublet (IAEA)
- Dr Dorothea Wiarda (ORNL)
- Dr Caleb Mattoon (LLNL)

- Dr Fausto Malvagi (CEA)

Meetings/events since GNDS-1.9 approved:

- **June 2019:** 31st WPEC - approved, figured out improvement process, made 2.0 branch - *last in person meeting*
- **May 2020:** 32nd WPEC - progress on 2.0
- **July 2020:** GNDS-1.9 Published
- **July 2020:** GNDS-1.9 Webinar
- **Dec. 2020:** Nuclear Data Week 2020 - status report
- **9-10 Nov 2020:** WPEC SG meeting - progress on 2.0
- **May 2021:** 33rd WPEC - final feature freeze, except for resonance issues
- **Aug. 2021:** mini-CSEWG - status report
- **20 Oct. 2021:** EG-GNDS Meeting - final approval on most open trackers
- **Nov. 2021:** Nuclear Data Weeks(s) 2021 – now
- **Dec. 2021:** Anticipate approval @ WPEC meeting, editing process begins
- **May 2022:** 34th WPEC - planned announcement of GNDS-2.0

What did we do the last two or so years?

GNDS-2.0 Highlights

- xsdir-like functionality: map file and checksum support
- Documentation markup: supports all metadata needed for DataCite.org DOI assignment
- Ground-up rewrite of TNSL
    - In collaboration with SG-42,48
    - Mixed elastic scattering
    - TNSL covariance
- Cleanups and bug fixes
- Full support for ENDF-6 data
- Met all SG-38 requirements

New map file and new multi-group boundaries and flux file:

- Multi-group boundaries format uses GNDS node to store the label and boundaries for a group.
- Flux stored as f(T,E,mu) using a GNDS 3d function.

Metadata requires a longer discussion:

- There are 4 sources of metadata schema between OSTI and DataCite.org
- Many of the markups are being adopted(adapted?) for GNDS-2.0
    - authorship vs. contributor - give proper credit for level of work
    - dates - much broader set of events than ENDATE, RDATE, DDATE and EDATE
    - relationship - which set is related to what other set and how

Dave Brown believes adopting these markups in GNDS and the metadata schema can relieve many stressors within CSEWG!

Problem #1: Giving credit where credit is due

Problem:

- The ENDF-6 format does not have enough space for all the authors
  - Overflow must be listed in free-text fields with unclear rules both for credit and formatting
- The ENDF-6 format does not have scheme for denoting smaller (but still important) contributions
  - These must be listed in free-text fields with unclear rules both for credit and formatting

SOLUTION (PARTIAL)

- Assigning proper credit:
  - <authors> - list of authors & affiliations of whatever length is needed
- Capturing minor changes:
  - <contributors> - list of contributors with nature of contribution ()
  - <dates> - list of dates with nature of data ()

ENDF Discussion: What Criteria Elevates a Contributor to an Author? What is the order for Authors? (My thoughts below)

- Bug fixes -> Contributor
  - Includes fixing normalizations, threshold energies, typos
- Major changes to evaluation -> Author
- Lead author/Creator/PI -> Authors please figure it out
- Lead author should be negotiated by the authors and the CSEWG executive committee if it is not clear or if there is disagreement
- Order of authors should be handled in similar manner

Problem #2: Meager explanation of versioning within an ENDF file

PROBLEM:

- Within an ENDF file, changes denoted with ENDATE, NMOD and the dictionary
  - We very rarely remember to change them
  - Most of us don't know how to use them correctly

SOLUTION (PARTIAL)

- <dates> markup lets us denote important dates in an evaluation lifecycle
  - DataCite defines many useful dateTypes: accepted, available, submitted, updated, etc.

- <date dateType="accepted">…</date>

Problem #3: How sets are related to one another?
PROBLEM:

- The ENDF-6 format does not denote which file is derived from another. LDRV just flags that a file is derived.
- GNDS provides evaluated and derived styles and a "derivedFrom" link. This solves the problem within a GNDS file.
- How do I denote the ENDF->GNDS connection? The ENDF->ACE connection?

SOLUTION (PARTIAL)

- <relatedItem name="…" href="…" relationType="…" />
- DataCite defines the following relationTypes:
  - 'IsCitedBy','Cites','IsSupplementTo', 'IsSupplementedBy','IsContinuedBy', 'Continues', 'Describes', 'IsDescribedBy', 'HasMetadata', 'IsMetadataFor', 'HasVersion', 'IsVersionOf', 'IsNewVersionOf', 'IsPreviousVersionOf', 'IsPartOf', 'HasPart', 'IsPublishedIn', 'IsReferencedBy', 'References', 'IsDocumentedBy', 'Documents', 'IsCompiledBy', 'Complies', 'IsVariantFormOf', 'IsOriginalFormOf', 'IsIdenticalTo', 'IsReviewedBy', 'Reviews', 'IsDerivedFrom', 'IsSourceOf', 'IsRequiredBy', 'Requires', 'Obsoletes', 'IsObsoletedBy'

Coherent elastic: bulk scattering off crystalline materials

- Outgoing angular distribution consists of delta functions at various mu_i
- TODO: sample angles directly using $s_i(T)$
  - Requires some work in GIDI+

The hierarchy for storing TNSL data was overhauled between GNDS-1.9 and GNDS-2.0
GNDS-2.0 layout integrates TNSL with all other reactions. Integrating and renormalizing TNSL double-differential cross sections produces a standard cross section and outgoing neutron distribution.

GNDS easily handles new LTHR=3 (mixed elastic) format proposed by M. Zerkle

- Some materials require both coherent elastic and incoherent elastic (plus inelastic) to properly represent thermal scattering region.
- Handled in GNDS simply by adding another **reaction** node for the new elastic term
- Example files for ^{7}LiH and ^{7}LiD were translated to GNDS and processed with FUDGE
  - Results can be translated to ENDL, ACE coming soon once we check latest format update…

Incoherent inelastic is trickier, often requiring extrapolation beyond tabulated S_{ab} grid especially at forward angles.

- A_0, M_n, $sigma_{bn}$, Sn(alpha,beta,T) are tabulated

- alpha,beta grids in many evaluations aren't sufficient for spanning all (E, E', mu) of interest
    - Short collision time (SCT) approximation is appropriate for large a,b but generally not as a approaches 0
    - Extrapolation required for small a, but appears to be handled differently by processing codes
        - Especially relevant for forward scattering where E' ≈ E

SPECIFICATIONS VS. REQUIREMENTS VS. ENDF-6

GNDS VS. ENDF-6

- All MF/MT's in ENDF-6 manual have GNDS analogs
- All low level formats in ENDF-6 are either obsolete or have GNDS analogs
- Developed 4 page summary showing connection between ENDF-6 and GNDS.
- Suggest making it an appendix to specifications
- TO DO: detailed (LIP/LAW/ whatever level) comparison between formats

GNDS VS. SG-38 REQUIREMENTS

- Approved map/library/xsdir/etc file markup
- Proper treatment of EOS in TNSL data
- Some elements of atomic data
- Improved FPY markup
- Processed data types
- Radiation damage
- dE/dx
- Resonance things: Brune transform, CP RRR
- Improved TNSL markup (see proposal/TNSL)
- Improved documentation markup (see proposal/documentation)
- Support for the sandwich formula (see proposal/sandwichProduct)
- TO DO: detailed comparison between format and each requirement sub-bullet

Generally unwise to force format discussion until we see what evaluators can provide & see what users need

We'll be editing the specifications for a while, which is required for final preparation of document

- Passive voice is required in all OECD publications
- British, not American spelling
- Discussion point -> Tracker conversion
- Many, many branches
- Many unclear formulations remain (e.g. interpolation)
- Update appendix with changelist

Implementation status? See talks from LLNL, LANL, & ORNL

What's next:

- Expect major format changes post-GNDS-2.0:
  - Synchronize nuclear structure formats with ENSDF as part of ENSDF modernization
  - Revamp uncertainty/covariance to make more ML friendly
  - Atomic data additions
  - FPY formats per FIRE collaboration recommendations
- ENDF to GNDS transition:
  - ENDF/B-VIII.0 released in GNDS-1.9
  - ENDF/B-VIII.1, JEFF-4, TENDL to be released in GNDS-2.0
  - Expect at least next release to be in both ENDF-6 and GNDS formats
  - Transition is slow; we must walk together and we can only go as fast as the slowest among us

Dave Brown is stepping down as EG GNDS chair once 2.0 is out the door

ENDF-102 Status Report
Dave Brown

Very quick ENDF-102 Update

Big change to manual:

- It builds correctly
- For the last two years, the build was broken and no one noticed
- The CI/CD system is down while we figure out configuration issues for Kubernetes
- The latex files also had dependencies on many style files included in the source that fought with system versions

It appears all Merge Requests are ready to go

- !13: Resolve "Add proper CONTRIBUTING.md file that describes how to make format proposals" https://git.nndc.bnl.gov/endf/format/endf6man/-/merge_requests/13
- !6: Replace Fmts-07.tex to implement mixed elastic scattering format proposal. https://git.nndc.bnl.gov/endf/format/endf6man/-/merge_requests/6
- !9: Resolve "FORMAT PROPOSAL: ENDF-102 Clarification for Primary Discrete Gammas" https://git.nndc.bnl.gov/endf/format/endf6man/-/merge_requests/9

Ready to be merged, Mike Dunn will do that

Missing Merge Requests for 3 recent proposals:

- #128: FORMAT PROPOSAL: Extend Kalbach-Mann formalism for deuteron breakup

- #112: Angular distribution of nucleon emission from deuteron breakup reaction
- #123: Format change to use MT=261 for neutron fields in special purposes libraries.
- #114: Format proposal defining KRL flag
- #113: Format change to include Brune parameters

Andrej Trkov mentioned: MT261 reserved for neutron spectrum fields for dosimetry

Format proposal process modeled on old ENDF-6 manual process, updated for git

- **Required:**
  - Issue tracker containing need & rationale for format
  - Merge request implementing manual changes (this is complex, see next slide)
  - Review of merge request handled using formal process
- **Preferred:**
  - Example file
  - Reference implementation in processing code

CONTRIBUTING.md file describes the process

The bug fix process is the format proposal process with quick informal review
Is the community OK with this process, or must it be more formal?

- **Required:**
  - Issue tracker containing need & rationale for bug fix
  - Merge request implementing manual changes
  - Review handled by chair or chair+helpers for more complex fixes

Quick edits to the CONTRIBUTING.md file can describe this process

Session: Covariance Committee

Adjustment

Updates from the covariance session committee
14:45 - 14:50
Dr Denise Neudecker

Updates from the Covariance Session Committee

The CSEWG covariance session template paper was submitted on June 8, 2021 to journal, containing templates for the following observables and corresponding leads:

- Total cross sections (A. Lewis)
- Capture cross sections (A. Lewis)
- N-induced charged-particle cross sections & angular distributions (D. Neudecker)
- Prompt fission neutron spectra (D. Neudecker)

- (n,xn) cross sections & angular distributions (J. Vanhoy & R.C. Haight)
- Average prompt fission neutron multiplicity (D. Neudecker)
- Fission yields (E.F. Matthews)

Adjustment: CSEWG will not publish adjusted VIII.1, BUT there is interest in adjustment results from the community.

VIII.1: one general-purpose library with mean values tuned by hand to reproduce selected integral responses, covariance remain unchanged. It is up to the users to do their own adjustment.

Into the future:

- Discuss adjustment in covariance session to give recommendation how adjustment could be done by users & warn users of caveats, learn where nuclear data could be improved,
- Might document some VIII.1 tweaks & integral data used,
- Work with validation session to agree on what benchmarks/ integral responses we use for tweaking, e.g., version of Jezebel, but also vet what integral responses are adequate for tweaking.

Other focus points for the release for VIII.1:

- Stringent testing of covariances before their release:
    - We will have continued discussions on progress on releasing new covariances,
    - It would be great if covariances could be fully processed before their release,
    - We should consider aiming for testing covariances (for mathematical consistency, see if uncertainties are reasonable) before release.
- Missing covariances: please let me know if there are any covariances missing to satisfy covariance needs of your institution. We will collect those needs.

Outline of covariance session reflects that:

- Talks on adjustment and needed sensitivities,
- New covariances coming in for VIII.1,
- New developments in:
    - Testing & processing,
    - Neutron-Gamma correlations,
    - Uncertainty quantification,
    - Methods development.

WPEC/SG46 TAR exercise: preliminary results
14:50 - 15:05
Oscar Cabellos

Target Accuracy Requirements:

- Legacy work in WPEC/SG26 (2005-2008):
  - established data priorities for uncertainty reduction in GEN-IV reactors.
  - The Target Accuracy Requirements (TAR) exercise:
    - Used BOLNA covariance matrices
    - Energy structure: "**15 energy groups** (based on physical considerations)"
    - No-correlations in energy, reactions and isotopes are considered **in TAR exercise**
  - **14 HPRL entries based on SG26 studies!**

- WPEC/SG46 (2019-2021):
  - Goal is to provide **updated target accuracies for nuclear data uncertainty reduction**
  - New reactors concepts are explored besides Gen-IV, MA burners, and ADS: MSR, SMR, micro reactors, and test reactors
  - **TAR** based on:
    - New covariance data matrices: ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0u
    - Using correlations in energy, reactions and isotopes
    - Energy structure: "7 energy groups (based on physical considerations)"
  - HPRL will be updated

  - **Target Accuracy Requirements for multi-physics processes:**
    - Target Accuracy Requirements (TARs) represent wishes and acceptance limits established by designers and/or assessors
    - Sg46 task: to establish TARs for Nuclear Data libraries
    - Approximately separating impacts due to reactor physics and due to other physics: combining sampling and linearized response (sensitivity) studies
    - Sampling-based back-propagation with reduced (adjusted) ND uncertainties

  - **TAR Methodology -** the **"inverse problem":**
    - To define the TAR on design parameters: R_n^T
    - To find out **<u>the required reduction in the cross-section uncertainties:</u>** Δx_i .
    - Different sets of cost parameters (lambda) related with each cross-section are defined and minimized

    - **Stake holders in TAR exercise:**
    - **Differential measurement experts**
    - **ND Processing**
    - **ND Evaluators**
    - **Reactor Designers**
    - **Reactor Physicists**

- **Benchmark Specifications: WPEC/SG46 Exercise on Target Accuracy Requirement (TAR)** *WPEC/SG46, May 2021,* https://oecd-nea.org/download/wpec/sg46/

Processing Covariances

- NJOY2016.63 with some processing issues
- Work in progress: AMPX –NJOY processing and comparison
- Issues in evaluated files, ENDF/B-VIII.0
  - Large procesed uncertainties (> 100%), e.g. B10(n,n')
  - Lack of ND covariances, e.g. no MF33 in Fe56, no MF34 in B10, no MF35 in Pu241
  - Processed null, e.g. Pu239(CHI)

- Reference:
  - M. Salvatores et al., "OECD/NEA WPEC Subgroup 26 Final Report: Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations", OECD/NEA/Nuclear Science, 2008.

Preliminary TAR results for new reactor systems in WPEC/SG46:

- ASTRID (600 MWe SFR, MOX fuel)
- ESFR-SMART (1500 MWe, SFR, MOX)
- **J-SFR750** (750 MWe, SFR, MOX)
- ALFRED (125 MWe lead-cooled fast reactor, MOX)
- UQ performed for above systems with sandwich formula and using the full ND covariance matrix from ENDF/B-VII.1, ENDF/B-VIII, JEFF-3.3, JENDL-4.0u
- No correlations vs. correlations: The impact of correlation terms is very significant in TAR assessments evaluation and produces very stringent requirements in ND
- Results for ENDF/B-VIII
  - many uncertainties are greater than target
    - results in keff uncertainty up to 5 times of target

- **1st Phase: Definition of TAR**
  - So far, ALFRED, ASTRID, ESFR-SMART and JSFR
  - **More reactors + sensitivity profiles: SMR, MSR, …Other systems ?**
- **2nd Phase: Uncertainty Quantifications**
  - Different libraries and associate covariance data (e.g. ENDF/B-VIII.0)
  - Assessment of 7-energy groups
- **3rd Phase: Performing TAR with inverse approach**
  - 7-energy groups
  - Correlation and no-correlation
  - Different set of cost parameters

One system and all parameters: e.g. JSFR

Mike Herman asked about cross-material correlation and Oscar said they included all cross-correlations.

The benefit of adjusting with criticality and reaction rate data
15:05 - 15:20
Robert Casperson

The benefit of adjusting with criticality and reaction rate data

Criticality and reaction rates

Critical assembly keff is sensitive to fission and scattering, so adjustment with keff creates correlations between those reactions.
Assembly neutron spectrum depends on PFNS and scattering properties.
Adjusting with fission ratios measured in critical assemblies can help constrain the fission cross section and assembly neutron flux.
— keff adjustment alone does not do this.
— These fission reaction rates are sensitive to the neutron spectrum, and are referred to as spectral indices.
— Measurements were quick, which allowed for multiple fission chambers and foil thicknesses. (Avoided some pitfalls of differential fission ratio measurements)

The ENDF/B-VIII.0 Spectral Indices Table

- most values are low when reading table
- For many assemblies, reaction rates systematically low by ~2%; all are ratios to 235U(n,f).
- This raises questions about validation of ENDF/B-VIII.0 major actinides.

Adjustment method

- There are several methods for adjustment, but we have used a hybrid of Monte Carlo sampling and sensitivity analysis for the regression (GLS).
  - Monte Carlo sample phases are decorrelated, which requires covariance rank + 1 samples.
  - Sensitivity vectors found in joint evaluation/integral model covariance matrix.
  - Variations include PFNS covariance, but currently not elastic angular or inelastic spectral covariances.
- Assembly and foil nuclear data varied together, to account for uncertainty in assembly neutron spectrum.

Impact of adjustment on integral data

- Adjustment includes keff and reaction rates, so resulting evaluation consistent with both.
- The collection of integral data from the ENDF spectral indices table is statistically significant enough to cause substantial changes in differential evaluation.
- Some 252Cf(sf) data supports the changes on the following slides, but there is not as much data available.

Adjustment impact on 235U and 239Pu differential data

- Confidence bands are reduced
- U235 fission down 0.9%, maintains criticality, impacts neutron spectrum
- Pu239 fission uo 0.7%, maintains criticality, impacts neutron spectrum

Benefits of adjusting with keff and reaction rates

- Adjustment can help address spectral indices validation issue.
- Adjusted fission and inelastic scattering uncertainties are reduced, resulting from combination of fission data, spectral sensitivity, and criticality data.
- Impact not sensitive to keff uncertainty; just as significant when all are set to 0.3%.
- Allowing adjustment with integral data could lead to novel and impactful future experiments.
- Confidence bands are reduced for 235U(n,f) and 239Pu(n,n').

Adjusted correlations between isotopes

Adjustment with pulsed spheres

- Spectral indices can impact modeled pulsed sphere nToF spectra.
- Pulsed spheres have more resolved measurements of neutron spectra but would require covariance matrix for nToF spectrum.
- Simulations of neutron detector have shown threshold variability between measurements which would need to be accounted for in covariance matrix.
- Adjusting to just two points with Pu pulsed sphere nToF spectra has a big impact on 239Pu(n,n') and PFNS

Path to adjustment

- Adjustment would require evaluated integral data with realistic covariances.
  - The single bad data point from the ENDF/B-VIII.0 spectral indices table would have doubled the impact on 235U(n,f).
  - Criticality and spectral indices seem like a good starting point, but smaller number of assembly materials preferred.
- Cross validation would help identify deficiencies of adjusted libraries.
  - Adjusting with subsets of data and validating with data left out would help users understand appropriate uses and shortcomings of these adjusted libraries.

- Pulsed spheres may be more sensitive to scattering uncertainties than reaction rates
    - Adjustment with pulsed sphere spectra complicated and covariance matrix not provided with data.

Getting sensitivities for various integral responses supporting nuclear data validation and adjustment
3:20 PM - 3:35 PM
Denise Neudecker
Jesson hutchinson

This a LDRD project

EUCLID uses and developed tools to get sensitivities for various different measurement
Different measurement types give complimentary data which can help to disentangle compensating errors and improve overall validation of nuclear data.

Using existing sensitivity tools to obtain a diverse collection of sensitivity profiles
• Brute-force sensitivities with FRENDY/SANDY
− Direct modification of ENDF/ACE files
− Requires individual isotope-reaction-energy perturbations and independent MCNP calculations
− O. Cabellos and A.R. Clark computed pulsedsphere sensitivities with this methodology*
• SENSMG
− Tool wrapped around the LANL deterministic transport code PARTISN
− Requires using multi-group cross sections
− Computed reaction rates, spectral indices (J. Alwin), and subcritical multiplication (A.R. Clark) sensitivities BeRP Subcritical Multiplication Fission Cross Section *D.Neudecker, ANE 159, 108345, (2021). Fission Spectrum Tools for sensitivities of different responses

Deriving and computing more sensitivities through existing capabilities
Using keff sensitivities, T. Cutler, J. Hutchinson, N. Kleedtke have derived and simulated other response sensitivities

- Beta-effective
- Reactivity coefficients
- Rossi-alpha

M. Rising developed new fixed-source sensitivity in MCNP for easier execution and faster run-time
• Central difference, brute force calculations (FRENDY/SANDY codes) − Difficult to distinguish Monte Carlo statistics from small perturbations − Computationally expensive • Differential operator (PERT card) − More complicated to use (many input cards needed = isotope x reaction

x energy) − Limited to reactions (no multiplicity, spectrum or angular distributions) • Adjoint-weighting (new FSEN card) − Easy to use with accurate results (like KSEN) − Reactions, multiplicity, and energy / angular distributions all available

Verification of the new sensitivity methodology has been undertaken.
• Performing extensive verification to provide a robust and accurate capability − Comparison between FSEN and PERT
• Comparison between FSEN and central difference − Verification of FSEN using FRENDY results

Computational benefits of the new MCNP6 sensitivity methodology are promising
• FRENDY/SANDY vs. FSEN efficiency − Figure of merit § Measure of Monte Carlo calculational efficiency § § Average efficiency gain for fission reaction • PERT vs. FSEN efficiency − Computational cost is roughly equivalent − Pre- and post-processing of PERT results not automated − No optimization of the prototype FSEN capability (yet)

Human cost to use PERT may be higher with how easy it is to use the new FSEN capability

W. Haeck programmed FAUST tool that processes all different output formats into common json format.

- FAUST
    - Input / output processing of MCNP, SENSMG results
    - Handling of all sensitivity data for use in nuclear data adjustment and experiment design optimization
    - Common and easy to use JSON format support (new MCNP6 FSEN output also available in JSON)
  - Crater tool used to rapidly study impact of nuclear data changes on validation benchmarks

EUCLID Uses sensitivities for many use-cases. One use-case is adjustment: we can filter to and select from our diverse set of benchmarks for adjustment.

Adjusting to Jezebel we can explore the impact on nuclear data and the propagated prediction and uncertainties for Jezebel.

One warning (among many): adjusting to data with unaccounted for biases leads to unreasonable results.

As mentioned however, adjusting to data with unaccounted for biases leads to unreasonable results

Adding in a Gaussian process with tunable parameters to account for the bias uncertainty for long TOF mitigates this issue:

Summary
• EUCLID computed sensitivities of several integral responses to nuclear data,

• EUCLID leveraged existing tools, but new ones were also developed,
• EUCLID uses sensitivities for validation, finding where compensating errors could hide in our libraries, optimization of integral experiments and adjustment,
• We are happy to share our sensitivities after release and are establishing contact with the NEA about possible sharing these data through their tools to the community
Sensitivities are in JSON format.

CSEWG: Covariance Committee - New eval.

Covariance update from INDEN
15:45 - 15:55
Roberto Capote

INDEN (nubar) covariance update
U-235, Pu-239, U-233

- **https://www-nds.iaea.org/INDEN**
- nubar fluctuations for resonances: reintroduced in ENDF/B-VIII.0 for n+^{235}U. Fluctuations will be added for all major fissile nuclei.
- Missed experiment by Gwin et al (1986) in 235U ENDF/B-VIII.0 nubar 500 eV-10 MeV: Nuclear Science and Engineering, 94, 365-379 (1986)
- Data for U-233, U-235, Pu-239 with uncertainties !!
- Relative to Cf-252 prompt (TNC), most of the uncertainty comes from Cf
- Fissile nubar uncertainties are of the order of ~ 0.5% in the range between 500eV and 100keV, for all fissile nuclei (U-233, U-235, Pu-239).
- Uncertainties reduced from 2% down to 0.5% in range 20eV-50keV (U-235, Pu-239, U-233):

Covariance update for light elements
15:55 - 16:05
Dr Mark Paris

- Covariance update for light elements
- Parameter uncertainty from Chi-square: The Old Way gives too-small uncertainty
- Uncertainties from chi-squared minimization: Nuclear Data Sheets 123 (2015) 165-170
- Example covariance
    - 17O system

        - (n,el)
        - correlation matrix
            - elements (-1.0,1.0)
- Covariances for ENDF/B-VIII.1, Anticipated; time-permitting:
    - CP induced
        - p-001_H_001.endf
        - p-002_He_004.endf
        - d-002_He_003.endf
        - t-002_He_004.endf
        - a-006_C_013.endf
    - n induced
        - n-003_Li_006.endf
        - n-004_Be_009.endf
        - n-008_O_016.endf

Q: Have you looked into the scaling by number of data points?
A: No

Covariance update for actinides in the RRR
16:05 - 16:15
Dr Marco Pigni

Evaluated Data for Fissile Actinides in the Resolved and Unresolved Resonance Region and their Coupling to Neutron Multiplicities

Overview:

- 233U
    - Motivation: underestimated reactivity for critical assemblies
    - Status: updates to PFNS, thermal constants, R-matrix improved subset of benchmarks1
    - RRR: extension up to 2 keV and inclusion of possible newly measured capture data
    - URR: relevant to assess impact on benchmark calculations in the energy range 2–40 keV
- 235U
    - Motivation: investigation on reactivity rates related to depletion calculations
    - Status: 238U evaluation (see Capote/Trkov presentation) affecting the burn-up trend
    - URR: updated evaluation by including recently measured fission data
- 239Pu
    - Motivation: R-matrix analysis to include TNC values (STD 2017) and PFNS (IAEA+LANL)

- Status: partial work to extend RRR up to 5 keV
- Neutron multiplicities: updated evaluation with fluctuations and related covariances in progress

U(nresolved) R(esonance) R(egion) ANALYSIS OF 235U:

- Except for the inelastic channel (11%), scaling factors ranging up to 6%
- Except for fluctuations, reasonable agreement with ENDF/B-VIII.0 (file 3)
- 20 keV is an acceptable upper energy limit for URR fit to account for self-shielding effects
- ENDF/B-VIII.0 evaluated data show fluctuating behavior (to be checked if there is formal consistency between file 2 and file 3
- Inelastic channel deviates from ENDF/B-VIII.0 below ≈10 keV
- μbarn should have no impact on criticality!
- Next step is the inclusion of fluctuations! (Resonance parameters ⇒ fit ⇒ effective/theoretical cross sections)

NEUTRON MULTIPLICITIES: On the (n, γ f) reaction

- Fluctuating behavior of prompt neutrons based on the competition of (n, γ f) and direct fission (n, f) processes
- The resonance fission widths for each level are used to calculate the partial energy-dependent fission cross section:
    - For 239Pu (having spins J = 0 +,1 +), the parameters used in the calculations are four

NEUTRON MULTIPLICITIES OF 239Pu:

- Measured data with different resolutions. Data from Ryabov seems to be the most consistent
- AS expected the correlation matrix reflects the nubar fluctuating behavior
- To reduce size of covariance matrix, energy grid properly defined around each energy level
- Calculated uncertainty is about <= 0.3%

Covariances for the Fission Product Yield Reevaluation
16:15 - 16:30
Amy Lovell

Covariances for the Fission Product Yield Reevaluation

Current status of fission product yield covariances:

- Uncertainties but not correlations are currently included in ENDF! (For both independent and cumulative fission product yields.)
    - There is also no format for the FPY covariances.
- The NA-22 funded re-evaluation project of the FPYs will include generating covariances.
    - New modeling capabilities (e.g., the LANL-developed, deterministic, Hauser-Feshbach code BeoH) and experimental measurements make it a prime time to perform this reevaluation.
    - Previous ENDF evaluations were based solely on experimental data and conservation/summation rules.
    - A.E. Lovell, T. Kawano, et al., PRC 103, 014615 (2021)
    - S. Okumura, T. Kawano, et al., arXiv:2102.01015 [nucl-th] 1 Feb 2021, in press JNST, LA-UR-21-20820

Model calculations and optimizations are used to produce covariances between fission products:

- Parameter and observable covariances are straightforward to calculate using a Kalman filter optimization (input of model parameters and baseline calculations plus experimental values and covariances)
- Observable covariances are calculated from parameter covariances and model sensitivities
- Covariances depend on the model parameters included in the optimization
- Covariances can be calculated between pairs of FPYs and incident energies
    - Cross-energy correlations for a single cumulative FPY and Correlations between FPYs for a fixed incident energy were shown for 239Pu(n,f). Example plots were given for 147Nd and cross-material covariances for Einc=0 and 5 MeV.

Future work:

- Cross-observable correlations are accessible, along with cross-target correlations
- Multi-chance fission input correlates compound nuclei along an isotopic chain (e.g. fission barriers for 236U, 235U, 234U, 233U enter 235U(n,f) calculations up to 20 MeV)
- Along with FPYs, prompt and delayed nubar are calculated consistently, providing further parameter constraints

Summary and comments

- Covariances between fission product yields will be available in ENDF as a part of the FPY re-evaluation, based on model calculations (provides a connection to decay data as well as all conservation rules included explicitly).
- The format of these covariances is not determined, and there is probably room for a compact format due to the lack of correlations between many FPYs.
- Are energy-dependent correlations important/useful?
- How can we validate these new covariances?

Andrej suggests to define the format in terms of the correlation matrix.

Ian Thompson says he is surprised to not see some cross-correlations. Amy explained that these results are still preliminary and do not include for instance ratio data.

Recent Work on Thermal Scattering Covariance Generation and Compression
16:30 - 16:45
Aaron Tumulak

Table of Contents
1 Introduction
2 SCALE Implementation
3 Data Compression Data Generation Principal Component Analysis Reconstruction Error
4 Conclusions

Motivation

- How is a quantity f affected by uncertainty in x1, . . . , xN?
- Expand f
- Treating x1, . . . , xN as random variables, we have f as a weighted sum of random variables with variance
- The partial derivatives are sensitivities and Cov (xi , xj) is the covariance between xi and xj.

The Sandwich formula:

- End users compute sensitivities.
- Evaluators provide covariances .
- The Evaluated Nuclear Data File format, ENDF-6 [1] provides file formats covariances for some types of nuclear data.

Thermal Scattering: Incoherent Inelastic Scattering

- At energies (approximately less than 5 eV), thermal scattering takes place.
- The thermal scattering kernel S (α, β) is two dimensional data. The double differential scattering cross section σ (E → E ′ , μ) is actually three dimensional data.
- ENDF-6 does not currently specify a format for storing S (α, β) covariance.

Generalized Nuclear Data Format:

- New data format [2] to eventually supersede ENDF-6
- Previous work developed a format in the Generalized Nuclear Data format for storing S (α, β) covariances.

SCALE Implementation

- Implementation performed in AMPX [4] at GNDS Data Structures Level.
- Covariance for S (α, β) data is four dimensional.
- α and β indices are flattened to a linear index.
- Underlying data structure is a symmetric two dimensional matrix.
- The base class Covariance is not necessarily symmetric to account for cross-covariance across different reactions.
- Existing classes updated to inherit from common base classes.

Generating S (α, β) Covariance Data:

- Covariance data was generated from 1000 random realizations of H in H2O.
- Full covariance matrix had (182 × 259)2 ≈ 2 × 109 entries.
- Full uncompressed covariance matrix occupied about 17.78GB of storage as HDF5 file.
- GNDS format supports more than just α, β parameters. Adding one more dimension with just 10 points brings data storage into TB range.
- GNDS format supports basic compression methods. Sparsity and symmetric are immediately applicable.

Conclusions

- Data structures for representing thermal scattering kernel covariances were implemented in AMPX.
- Covariance matrices will be quite large for practical problems.
- GNDS format already supports some methods of compression.
- Principal Component Analysis can take advantage of large singular values to further compress matrices.

Future Work

- Generate temperature dependent S (α, β,T) from perturbed probability density of states.
- Compute sensitivities for a benchmark problem.
- Propagate uncertainties in S (α, β,T) through benchmark problem.
- Quantify uncertainty due to uncertainty in S (α, β,T).

References

- M. HERMAN, "ENDF-6 Formats Manual Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII," BNL-90365-2009, Brookhaven National Laboratory (BNL) National Nuclear Data Center (2009).
- WPEC Subgroup 38, "Specifications for the next generation nuclear data hierarchy," 2016.
- G. TUMULAK, H. PARK, V. SOBES, W. S. YANG, and B. C. KIEDROWSKI, "Progress on the Development of Thermal Scattering Covariance Formats and Processing Tools," Trans. Am. Nucl. Soc., 121, 1354 (2019).
- D. WIARDA, M. DUNN, N. GREENE, C. CELIK, and L. PETRIE, "AMPX-6: A Modular Code System for Processing ENDF/B," ORNL/TM-2016/43, Oak Ridge National Laboratory (2016).

Update on Covariance Data Testing Strategy at LANL
16:55 - 17:10
Nathan Gibson

Towards an ENDF/B-VIII.0-based Covariance Library

- Processing through NJOY's ERRORR module
- Identifying and correcting mathematical and physical deficiencies
- Communicating across pipeline, from evaluator to end user
- Understanding use cases and interpreting results Releasing to customers

Motivation for Library
- Criticality Safety
  - Whisper code
  - Safety limits
- Experiment Design
  - EUCLID project
  - Validating data and detangling compensating errors
- Uncertainty Quantification
  - Sensitivity-based approaches ("sandwich rule")
  - Sampling-based approaches (stringent requirements, distributions)

Challenges of Library Creation

- Processing
  - Covariance data has matured since NJOY development
  - Code assessment and changes
- Baseline
  - No complete in-house past work
  - No well-understood benchmarks

- Looking to outside work
- Data Deficiencies
    - Mathematical (negative eigenvalues, etc.)
    - Physical (comparison to experimental unc., etc.)
    - Incomplete data sets

Need to develop testing framework!

Approach to Testing

1. Interaction
2. Processing
3. Checks
    a. Mathematical properties
    b. Constraints
    c. Physical bounds
4. Error propagation

Notes:

- This presentation is on strategy and building infrastructure, not results.
- Work first motivated by ENDF/B-VIII.0 but will be used for ENDF/B-VIII.1 betas.
- Looking for community feedback for collaboration.

Interaction

Needs:

- Parse ENDF-formatted covariance data
- Build super-matrices from sub-matrices
- Identify what data is available in an evaluation

Interaction: ENDFtk

Processing

NJOY/ERRORR:

- Robust and powerful but predates modern covariances
- Errors: evaluation or NJOY?
    - Examples: Fe-54, O-1 6
- QA checks
    - Consistency between relative and absolute
    - Running on evaluation grid
    - Processed values between evaluation values

Checks: Mathematical Properties

- Requirements
    - Positive definite
    - Symmetric
    - Correlations in [-1, 1]
- Gray Areas
    - Large relative uncertainties
    - Implied asymmetric distributions
    - Roundoff issues

Checks: Constraints
Summation:

- Normalized quantities stay normalized (e.g., PFNS)
- Total is sum of partials
    - NI-type
    - Overspecification
    - Missing channels

Tough Questions:

- What can be fixed during library generation?
- What requires rejecting an evaluation?

Checks: Physical bounds
Sources:

- Expert judgment limits set by D. Smith in: "Guidance on Generating Neutron Reaction Data Covariances for the ENDF/B Library"
- Lower limits defined by Neutron Data Standards uncertainties if a reaction is predominantly measured relative to a specific standard
- Limits defined by templates of expected measurement uncertainties
- Spread in differential data
- Physical Uncertainty Boundary method limits (Neudecker, EPJ N 6, 19 2021).

Useful warnings or "hard stop" errors?

Checks: Physical bounds

- Sanity check # 1:
    - Don Smith defined lower limits based on expert judgment given his experimental background.
- Sanity check # 2:

    - Compare to standards' unc. (e.g., most 239Pu nu-bar data measured relative to 252Cf)
- Sanity check #3:
    - Templates of expected measurement unc.
- Sanity check #4:
    - Compare against spread of experimental data (critical barrier: no easy access to curated data)
- Sanity check #5:
    - Physical Uncertainty Boundary method (work in progress)

Error Propagation:

- "Sandwich Norms"
    - Simple problems for A/B comparisons
    - Assess if processing-based changes have large impact
- Benchmarks
    - Propagate uncertainties to ICSBEP benchmarks, etc.
    - Previous work by ORNL
    - Goal: impact of new evaluations, consistency of independent efforts
    - Important: unadjusted covariances

Summary

- Motivations
    - Processed library for user applications
        - Sandwich rule and sampling
        - Continuous and MG
        - Fast and thermal
    - Test ENDF/B-VIII.1 betas as they are released
- Testing Approach
    - Interaction
    - Processing
    - Checks
        - Mathematical properties
        - Constraints
        - Physical bounds
    - Error propagation

Neutron-Gamma Emission Correlations in 252Cf(sf)
17:10 - 17:20
Ramona Vogt

Stefano Marin

Importance of Neutron-Gamma Correlations

- Give insight into the physics of the fission process
- Correlated neutron-gamma emission are a signature of fission, albeit small in magnitude
- Correlations introduce systematic bias in asymmetric and inefficient detection systems

Neutron-gamma correlations can arise because of:

- Fragment energy and angular momentum conservation
- Correlations between excitation energy and angular momentum

Going More in Depth: Covariance vs. E_n, $E_{g,}$ q_{ng}

Coincident counts are intimately related to the covariance. In the limit of single-particle detection:

$$W_{n\gamma} = \frac{D_{n\gamma}}{S_n S_\gamma} = C - 1$$

With

$$C = \frac{\mathrm{cov}\left(N_n, N_\gamma\right)}{\langle N_n\rangle\langle N_\gamma\rangle}$$

Expressing coincident counts in terms of a covariance allows for a much more in-depth and rigorous analysis:

- No multiplicity limitation
- Covariance and means display linear behavior
- Differential calculus of covariance

Conclusions:

- We have found evidence of neutron-gamma correlations in phase space. An enhancement of neutron-aligned, band-transition gamma-rays has been observed.
    - The findings were confirmed with an independent experiment on ^{252}Cf(sf). We have also observed a similar enhancement in ^{242}Pu(sf).
- The correlations are small (few %) but, for certain configurations of detector geometry and energy acceptance, can become significant (~10-15%).
- To better understand the physics of fission fragments giving rise to these correlations we are pursuing two simultaneous investigations:
    1. ^{239}Pu(n,f) to test the incident-neutron energy dependence of the correlations across a large energy range
    2. ^{252}Cf(sf) with fragment detectors to gate on the event-by-event excitation energy of the fragments.
- **S. Marin** et al. "Event-by-event Neutron-Photon Multiplicity Correlations In ^{242}Pu(sf)", *Proceedings of the Institute for Nuclear Materials Management* (2021).

Bayesian Monte Carlo evaluation framework for imperfect data
17:20 - 17:35
Goran Arbanas
Jesse Brown

Assumptions or approximations used with Bayes’ Theorem:

1. The model and the prior PDF of data are assumed to be perfect
2. The model is approximated by its 1st order (linear) expansion
3. Prior and posterior PDFs are approximated by normal PDFs.

- We recongnize that 1. is equivalent to constraining the posterior expectation values of delta, and of its covariance matrix, to 0
- We remove 1. by letting evaluator choose values of <delta>’ and Delta’
- 2. and 3. Can be removed by Metropolis-Hastings Monte Carlo

Overview of approximations used by ORNL codes

- Bayes’ theorem with arbitrary constraints
- GLS is recovered

Metropolis Hastings Monte Carlo (MHMC) Algorithm

Analytical solutions: Linear models

- The upper plot shows the perfect (within statistical uncertainty) agreement between the analytical and MHMC values for <z>’and <delta>’
- The lower plot shows that the difference between the analytical and MHMC <z>’ is not > 0.06% for any element of z.
- Diagonal of C’ matches analytical to within < 0.6%, off-diagonal requires more iterations
- Delta’ matches well throughout

Comparison to GLS

Application to RRR evaluation: U-233

- Fit 3 resonances allowing the energy eigenvalues and neutron widths to vary
- The explicit application of ⍰! = 0 gives the evaluator control over model/data defects (background, normalization, etc.)

- Uncertainty on model now envelopes the data

Uncertainty analysis: covariance and beyond

- 6 resonance parameters
- ~30,000 posterior sets make up PDF
- Posterior PDFs compared to GLS (black) and prior (black-dashed) PDFs
- Instead of storing covariance, store posterior sets
- All PDFs are positively skewed

Considerations

- BMC evaluation is a tool to address:
    - Imperfect data & models
    - non-linear models
    - non-normal PDFs
- fitAPI implementation validated with analytical solutions for linear models
- New posterior PDFs may need new storage formats to allow storage of non-normal PDFs
    - Storing posterior sets allows for: variance, covariance, skewness, etc.

An Uncertainty Quantification Toolkit for GNDS Formatted Libraries
17:35 - 17:45
Kyle Wendt

Evaluations with Means and Uncertainties (EMU): An uncertainty quantification toolkit for GNDS formatted libraries.

EMU is our toolkit for working with nuclear data covariances

- Suite for generating realizations of GNDS formatted nuclear data
    - Built on top of FUDGE for reading and writing GNDS
        - Library agnostic, only need a translator to/from/GNDS
        - Translator must also correctly translate covariance data.
- Manages the workflow for multi-material UQ studies
    - Generation of raw nuclear data realization
    - Processing of realizations into heated and grouped data
    - Feeding in multi-material variations into application codes
- Python scripting framework to make interaction with sampled libraries extremely simple.

EMU will use all available covariance data.

- Nuclear data libraries define cross section covariances as describing multivariate normal distribution (This is physically wrong)

Continuous covariance matrices are often interpolations

- In ENDL and ENDF-6 (the formats)
    - Computation via a coarse flat interpolation
    - Uncertainty is often computed via fine linear interpolation

EMU handles variations as efficiently as possible

- EMU exploits the linearity of Gaussian vectors
- And that the interpolations used can be written as linear operators:

EMU algebraically treats derived terms post variation

- Automatically correct if we change the underlying distribution of the variations, i.e., from normal to log normal, or some ML distribution

EMU is designed with future constraints in mind

- EMU is type driven, will handle new channels/reaction if they are encoded in GNDS types
- Pre-interpolation variation and algebraic evaluation minimize the dimension of each material's covariance matrix, will allow for efficiently sampled cross material correlations.

EMU managed workflow for multi-material UQ studies

- EMU "Sample Map" files defines a UQ study
- The map tag points to a source GNDS formatted library
- The processing tag enables automatic processing of sampled data through FUDGE scripts
- The variations tag controls how many variations will be made, and which reactions will be varied
- These files are parsed into a data structure that symbolically represents the study

EMU applied to Godiva K_{eff} calculations:

- Systematic structure allows EMU outputs to be readily incorporated into other workflow tools such as LLNL's Maestrowf minimal effort

Conclusion

- EMU is LLNL's new tool kit for generating realizations of GNDS formatted nuclear data
- Sample generation is treated extremely efficiently
    - Minimize underlying dimension of sampled space
    - Computing derived channels post-variation
- This efficiency will enable cross material correlations
    - Such as those resulting from adjustment to integral data.
- EMU also acts as a workflow manager
    - Generation to Application
    - Scriptable interface to access realized data and parameters
- Open source release targeted for some time in FY 22

Unifying the URR PT approaches and covariance work in a consistent framework
17:45 - 18:00
Matteo Vorabbi

Unresolved resonance region

- Thermalization of neutrons in 238U by elastic scattering requires ~ 2200 collisions
- Energy loss by elastic scattering in the URR amounts to ~ 240 collisions
- ~ 11% of collisions occur in the URR
- This is something we should care about
- Resonances are too narrow to resolve experimentally
- We cannot determine individual resonance parameters
- We can only determine averages of parameters
- Enough to determine the cross section PDF

Cross section probability distributions:

- The probability distribution is a measure of our ignorance of the cross section
- If we know the cross section exactly, the PDF is a delta function

We propose an alternative method:

- Standard:
  1. Sample cross section
  2. Doppler broadening
  3. Accumulate PDF
- Alternate
  1. Sample cross section
  2. Accumulate PDF
  3. Doppler broadening

How are these PDF's connected?

- A "history" in a reactor simulation represents many "real-world histories" (N >> 1010)
- Each "real-world history" is assumed to be statistically independent so the central limit theorem applies
- Our alternate approach is essentially an event-by-event PDF

What this means for the standard approach:

- We've rephrased URR PT construction as composition of probabilities:
  - target temp PDF
  - URR parameters
- Central Limit Theorem connects alternate(e-by-e) and standard URR PDFs

- We can combine other sources of information, namely experiment!

What this means for the alternate (event-by-event) approach: We can combine probabilities in any order we want

Without CLT, alternate event-by-event PDF is very broad and capture peak in wrong place (mean value still the same)

Average cross section:
The event-by-event PDF leads to an average cross section that is in disagreement with the one extracted from ENDF

Testing probability tables in V&V suite Poor initial results for ZPRs and BigTen now much improved. Because alternate (event-by-event) PDF is very broad and peaked in wrong place, it performs poorly in benchmarks

Combining theory and experiment: We can combine theory and experiment at zero temperature

PDF at 0 K for n- 238U:
- The experimental PDF is a strong constraint for the theoretical one
- The combined PDF (normalized) is very similar to the experimental one

Heating the PDF for n- 238U
- The variance problem seems to be solved! (we need to run some benchmarks!)
- We can combine experiment with either PDF variant!

Summary & outlook:
- A Bayesian approach is more advisable for the PDF calculation in the URR
    - Different probabilities are properly combined together
    - Including experiment is straightforward
    - Enables event-by-event treatment in URR
    - Traditional UQ method and traditional self-shielding method should be interchangeable
- Future work will be devoted to
    - Speed up numerical calculations of PDFs at higher temperatures
    - Fit the zero-temperature PDFs with a “universal” function

What if… We didn’t need to compute resonance ladders?

How can we fit the PDFs?

- We are focusing on neutron-induced reactions
  - Many target nuclei
  - Different reaction channels (elastic, capture, …)
- We are looking for a "universal" PDF for each reaction channel
- We used standard fitting procedures and also symbolic regression techniques to find a proper function 20 P(, E) = exp (X 6 n=0 pn(E) (ln) n)

Tuesday 16 November 2021

Session: Measurements Committee

LANL progress on ChiNu and Scattering
10:10 - 10:20
Keegan Kelly

LANL Updates on Chi-Nu and Neutron Scattering

Outline

- Chi-Nu Prompt Fission Neutron Spectrum (PFNS):
  - Revisit 239Pu
  - Updates on 235U, 238U, and 240Pu
- Neutron Scattering at LANL
  - Revisit n-γ technique with liquid scintillators
  - Results from carbon measurements
  - Extension to CLYC scintillators

Review of the Chi-Nu arrays

Recall 239Pu PFNS: Published in 2020

- Kelly, et al. PRC 102 034615 (2020)
- Kelly, Marini, et al. NDS 173 42 (2021)

235U PFNS: Results Finalized, Publication in Preparation

- Comparison with CEA results

- Kelly, et al. PRC in prep, was published in a preliminary form in NDS

238U PFNS: All DAQ Completed; Prelim. Analysis

- 238U to be finalized next year
- Able to consider comparisons of 239Pu, 235U, 238U, …, across wide Einc n range

Scattering: Liq. Scint. N-γ Coincidence Analysis

- γ-tag for Einc n and Eout n
- Good liq. Scint. timing reveals inelastic level structure
- Simple case: carbon – shown last year – also measured Fe and Pt
- Random coincidences are easily removed (O'Donnell, NIMA 805 (2016) 87)
- What are the backgrounds?

Backgrounds from γ-Anticoincident Neutrons

- The elastic scattering 12C(n,n) reaction is a likely source
- Do a simple Monte Carlo calculation for this background:
    - Sample incident neutrons from WNR FP15L flux shape
    - Calculate Eout n from sample Einc n , convert to TOFs
    - Vary TOFs according to random γ timing, recover new Einc0 n and Eout0 n
    - Fill histogram with counts = σ(Einc n)
- Possible to extract cross sections from this background?...maybe...

Extract n, γ, and Correlated n-γ Distributions

Corr. n-γ Distributions for Wide Range of Einc n

CoGNAC Array of CLYC Detectors for Scattering

Very Early Data from CoGNAC + Liq. Scint

Summary

- Scattering measurements this run cycle:
    - Al, Fe, and Be, with C for calibration
- CoGNAC array of CLYCs in progress
- More to come in the future!
- Chi-Nu Results and Future:
    - 239Pu PFNS full results published in PRC in 2020
    - 235U PFNS finalized and publication in progress
    - 238U full data set collected, and preliminary analysis has been applied
    - 240Pu(sf) PFNS collected with liquid scint.
- In-beam PFNS delayed due to PPAC delays and beam

Q: What has CEA measure for u5 and u8?
A: There's a new person to analyze u8, nothing in U5 yet

ORNL neutron induced cross section experiments on Zr90
10:20 - 10:35
Klaus Guber

GELINA
- Time-of-flight facility
- Pulsed white neutron source (10 meV < En < 20 MeV)
- Multi-user facility with 10 flight paths (10–400 m)
- Measurement stations have special equipment to perform the following:
    - Total cross section measurements
    - Partial cross section measurements

Neutron production:
- e- accelerated to Ee-,max ≈ 140 MeV
- (e- , g) Bremsstrahlung in U-target (rotating & cooled with liquid Hg)
- (g,n) , (g ,f) in U-target
- Low energy neutrons by water moderator in Be-canning
- NCSP-Y12 build a new neutron production target for GELINA

Capture cross section measurements at GELINA: Total energy detection principle
- C_6D_6 liquid scintillators
    - 125°
    - Pulse height weighting technique
    - Weighting function from Monte Carlo simulations
- Flux measurements (IC)
    - 10B(n,a)
    - 235U(n,f)
- L = 10 m, 30 m, and 60 m

Total cross section/transmission measurements

Oak Ridge National Laboratory measurement activities for Zr
- Zr has 5 stable isotopes; at least 4 major isotopes should be measured
- Good high-resolution Oak Ridge National Laboratory (ORNL) total cross section data for separated isotopes are available, even for the long-lived radioactive fission product

93Zr; data were retrieved from the Jack Harvey archive of ORELA experiments. Experiments were performed with metallic samples at 80 and 200m FP length.

- Therefore, only neutron capture experiments must be performed using isotopically enriched samples
- Transmission and (n,g) Experiments with natural samples have been performed at GELINA: list mode data sorted into time-of-flight (TOF) spectra for data reduction
- Natural sample data serve as a good sanity check of the ENDF files for separated isotopes
- The combination of the natural sample capture data with the total cross section of the separated isotopes will help to obtain parameters for the strong capture resonances even, without data from enriched samples
- Because travel was cancelled due to COVID-19, a contingency plan was devised with the European Commission (EC)Joint Research Centre (JRC) to perform experiments
- Raw experimental data will be acquired by JRC-Geel and shipped to ORNL, where all data sorting and reduction will be performed on ORNL computers
- A 90Zr metallic sample was produced by ORNL's Isotope Science and Engineering Directorate and shipped in September 2020 to JRC-Geel
- Capture and transmission experiments were performed in 2021

Old ORNL 90Zr data

- Resolved resonances are visible above 1 MeV by a factor of 3 more than previous experiments
- Total cross section of 93ZrO2 resolved resonances well above 100 keV

ORNL measurement activities for Zr

- Transmission experiments with different Zr samples were performed using the FP4 50 m station
- Experiments used different background filter combinations

90Zr sample

- Metallic samples are the first choice for capture experiments, as they help reduce backgrounds from sample scattered neutrons due to the lack of scattering compound material such as H,O and C
- The sample is not very uniform and is warped, but for capture experiments, this is not a real problem
- Transmission samples should be uniform, but with good ORELA transmission data, this is not an issue
- However, the nonuniform transmission data could be used to test analysis program data correction procedures; the results can be compared to existing ORELA transmission data

Background determination in transmission using black resonance filters

Comparison of 90Zr transmission to ENDF: Many deviations

Status of NCSP experiments at EC-JRC Geel

	W	Cu	Ca	Ce	V	Zr	La
Sample	Metallic disks 182,183,184,186 2009–2011	Metallic disks 63 and 65 2011–2012	Metallic disks Nat Ca 2013–2014	Metallic disks Nat Ce, Ce-142 oxide 2014–2015 2018–2019	Metallic disks 2015–2016	Nat Zr metallic disks $^{90,91,92,94}Zr$ 2016–2017	Nat La metallic disks 2017–2018
Experiments GELINA	60 m, 30 m (n,γ) transmission	60 m (n,γ)	60 m (n,γ) transmission	Nat Ce 60 m (n,γ) Nat Ce transmission, ^{142}Ce experiments completed	60 m (n,γ) transmission	Nat Zr 60 m (n,γ) + transmission ^{90}Zr transmission and (n,γ) data in FY2021	60 m (n,γ) transmission
Data sorting	Finished 60 m + transmission	Finished 60 m	Finished 60 m transmission	Finished for thin and thick sample, ^{142}Ce data sorting finalized	Finished for thin and thick sample	Finished for thin and thick natural sample, ^{90}Zr transmission	Finalized
Reduced to cross section	X-section, transmission	X-section	X-section transmission 0.6, 1.0, 5 cm samples	2 mm X-section 2 mm transmission 10 mm transmission ^{142}Ce data	Thin X-section 0.35 and 2 mm, transmission	^{90}Zr transmission	X-section, transmission
Data testing	Data ready for evaluation	Data ready for evaluation	Data ready for evaluation	Data ready for evaluation	In progress, data ready for evaluation	In progress	Data ready for evaluation
Analysis and evaluation	Finalized and submitted to National Nuclear Data Center	Finalized and submitted to National Nuclear Data Center	Finalized and submitted to National Nuclear Data Center	In progress Final stages	In progress		In progress

People supporting JRC experiments and evaluations:

- Peter Schillebeeckx, EC-JRC Geel
- Carlos Paradela, EC-JRC Geel
- Stefan Kopecky, EC-JRC Geel
- Jan Heyse, EC-JRC Geel
- Ruud Wynats, EC-JRC Geel
- Clint Ausmus, Mike Zach, ORNL
- Marco Pigni, ORNL
- Chris Chapman, ORNL
- Jordan McDonnell, ORNL
- Jesse Brown, ORNL

LANL progress on LENZ, SPIDER, and SREFT
10:00 - 10:10
Hye Young Lee

LANL experimental updates on LENZ, SPIDER and SREFT in FY21

Neutron-induced reactions on natural carbon at LANSCE:

- One systematic measurement from threshold to 20 MeV.

- Directly measuring a diamond detector with the white source neutrons at LANSCE, carbon acted as an active target, enabling to measure (n,p), (n,d), (n,a) reactions along with the observed yields to infer neutron elastic scattering reaction.
- Kuvin, Lee, et al. PRC 104, 014603 (2021)

Neutron induced reactions

LENZ @ LANSCE: Carbon active target to measure (n,p), (n,d), and (n,a) rxns and n elastic scattering, reveals improved data that differs from current standards:

12C(n,α_0)9Be_{gs}
13C(n,α_0)10Be_{gs} & 13C(n,n')13C
16O(n,α_0)
54Fe(n,p)
56,58, 59Ni(n,z)

SPIDER: 252Cf source w/ HPGe γ detectors

107Tc
Fission yields- thermal to 20MeV

SREFT Spatially resolved fission tracker, LANL-→ in progress

TPC, smaller, cheaper
252Cf preliminary data

Overview of Nuclear Data measurement and analysis at RPI
10:35 - 10:50
Prof. Yaron Danon

Outline

- Neutron capture in 54Fe (S.Singh)
- Thermal total cross section measurements (D. Fritz)
- Thermal neutron die-away measurements (B. Wang)
- Neutron capture measurements on ^{Nat}Ta, ^{238}U, and 235U (K. Cook)

Neutron capture in 54Fe

54Fe (n, γ) Measurement – Motivation:

- Fe is an important constituent in many nuclear systems
  - Reactor, fuel storage, radiation shielding applications
- Natural Fe and 56Fe cross sections have been studied extensively, but there is a lack of data available in EXFOR of the 54Fe(n, γ) cross section
  - 56Fe evaluation work has highlighted need for new measurements and evaluation for 54Fe
  - nTOF data from 2014 was recently added to EXFOR after measurements began at the RPI LINAC
- There are various discrepancies between different evaluated data libraries, where some resonances are present in one evaluation and not the other

Overview of C_6D_6 Capture Array:

- An array of seven C_6D_6 liquid scintillators surrounding the sample of interest at a flight path of 45m
- The system is designed to perform radiative capture in the keV – low MeV energy range
- All the detector structural materials have a low capture cross section to minimize neutron sensitivity
  - Materials are mostly thin Al
- System is based on the principle of the total energy method
  - Pulse weighting is required

54Fe (n, γ) Measurement – Prior Data:

- nTOF ^{54}Fe Measurement (2014):
  - ~0.007 at/b 99.7% enriched ^{54}Fe sample was measured at nTOF in 2014
  - High resolution data (185m flight path) taken
  - Normalized to saturated resonance in Au
  - How does RPI data compare to nTOF?
- RPI Natural Fe Measurement (2014):
  - Older version of keV capture system was used to measure a thick natural Fe sample
  - Analysis was focused on ^{56}Fe capture cross section
  - ^{54}Fe resonances are clearly visible in capture data
  - Is it possible to cross-normalize this measurement to ^{54}Fe data?

54Fe (n, γ) measured and calculated Yield

- nTOF resonance parameters seem to provide better agreement to RPI experiment than JEFF or ENDF resonance parameters
- Some missing resonances from JEFF evaluation can be clearly seen in RPI and nTOF experiments
- A new set of resonance parameters will be fitted to RPI data

Thermal total cross section measurements

New cold moderator (ETTC)

- Neutronics
  - Polyethylene
    - Large enough to cover collimation
    - As close to source of neutrons as possible
    - As cold as possible in a consistent fashion (Cooled to between 20 and 30 K)
  - Maximize gain over existing source (ETT)
  - Metric: Integral counts in 1 – 5 meV range
- System
  - High density polyethylene (HDPE)
    - < 30 K w/ 1.5 kW on target
    - Good connection to cryostat
  - Long cold finger: protect cold head from radiation
  - Large cold finger cross-sectional area
  - Portable; Minimal material; Can withstand High-Vacucum
  - Single Stage Cryo-cooler

Experimental gain verification

- After LINAC power normalization the ETTC achieves a gain up to 8 over the ETT
- ETTC extends the usable flux below 1 meV

Polyethylene total cross section

- Excellent agreement between ETT and ETTC cross section for polyethylene (PE)
- Good agreement between all RPI measured cross sections, other measured cross section, and evaluated thermal scattering libraries (TSL)
- Experimental error bars account for all statistical and areal density uncertainty

Polyethylene detailed comparison to ENDF/B-VIII.0

- High accuracy (~ 1%) measured total cross section shows differences when compared to the evaluation
- Overall, the evaluation is higher than the experiment
- About 2.8 % discrepancy near 0.01 eV

Polystyrene and Plexiglas total cross section

- Generally good agreement between measured cross section and TSL evaluation for polymers
- Differences in cross section between Plexiglas G and Plexiglas G-UVT
- Experimental error bars account for all statistical and areal density uncertainty

YHx total cross section

- Generally good agreement between yttrium hydride measured cross section and TSL evaluation for both concentrations
- Experimental error bars account for all statistical and areal density uncertainty
- Error bars on evaluation represent estimated uncertainty on H/Y ratio from samples

Thermal neutron die-away measurements

Motivation and setup

- Provide a low-cost experiment to validate the preference of Thermal Scattering Libraries (TSL).
- Use a DT source to pulse a moderator material and measure the thermal leakage
- Compare to (MCNP) simulations.

Raw data for water

- Enables measurement between 30-150 micro-seconds
- Room background is dominated by source return

Distilled Water Experiment

- Simulation
  - Source (Flux monitor data)
  - Sample (Water only, no beaker)
  - ^{3}He Detector
  - Air
  - No structures or Cadmium Shield
- Experimental Data shows good agreement with MCNP

Polyethylene Experiment

- Pulse discrepancy (0 to 25 μs)
- Simulation results show faster die away (steeper slope)
- Sources of discrepancies may be:
  - Higher total cross section shown before
  - Sample Crystalline structures (affects angular dependent scattering)

Neutron capture measurements on ^{nat}Ta and ^{238}U

RPI γ-Multiplicity Detector

- 16 segment NaI(Tl) multiplicity detector
  - Total volume: 20 L of NaI(Tl) surrounding the sample
  - Inside of the detector is lined (~1 cm) with a B_4C ceramic sleeve which is enriched 98.4% in ^{10}B to absorb scattered neutrons
  - Greater than 95% efficiency (compared to C6D6 which is less than 10%)

- Detector was used for capture yield measurements in 0.01 - 3 keV energy range
- Detector electronics was upgraded from analog to a 14 bit 250 Mhz Digitizer
- Upgraded system with digitizer. Goal to measure gamma spectrum

Thermal Capture Yield Measurement: ^{nat}Ta
- 10 mil thick ^{nat}Ta – 0.012% ^{180m}Ta
- Energy Range: 0.01 – 100 eV
- 10 mil natural sample: includes ^{180m}Ta & ^{181}Ta
- ^{180m}Ta evaluation is in JEFF only
- First-order calculated capture yield is shown for evaluations.
- New data not present yet in EXFOR

Shifted Ta-181 Resonance: 13.95 eV
- NNL/ORNL evaluation is in better agreement compared to ENDF and JEFF but still does not match the data

^{nat}U Thermal Capture Yield
- Sample thickness: 20 mil
- Sample mass: ~18.2 g
- Natural sample: 0.7% ^{235}U
- Validation of the new DAQ system and processing codes (Julia based)

^{238}U γ-emission energy spectra for a two-step cascade
- Compared to a measurement using the Detector for Advanced Neutron Capture Experiments (DANCE) array at Los Alamos Neutron Science Center (LANSCE)
    - J.L. Ullmann et al. Nucl. Data Sheets 119, 22–25 (2014)
- General agreement with the LANSCE shape
    - Sum of the low and high peaks is the neutron separation energy of 4.8 MeV

Summary
- A new capture measurement of ^{54}Fe will help improve resonance parameters
- Total cross section was measured for polyethylene, polystyrene, plexiglas and YHx
- Neutron die-away method was developed to provide data for validation of TSLs
- Neutron multiplicity detector improvements were validated with ^{238}U and provided new ^{nat}Ta capture yield in the thermal region
- It will take 2 years to build new equipment

Spectroscopy of fission products for forensics
10:50 - 11:00
Andrea Mattera

Experimental campaign: Background

- The most common way to identify fission products and determine their yield, is to measure the characteristic γ-rays emitted in their decay ("activation technique")
- This technique fully relies on a solid knowledge of nuclear decay data (i.e., γ-ray energy and intensities), as well as fission yields
- Experimental campaign to accurately measure decay data of selected fission products relevant to Nuclear Forensics

Previous Experience with Medical Isotopes

- A striking example of the sensitivity and the improvements to the decay schemes that can be achieved with modern arrays is given by 86Y β+ -decay
- Our study identified 52 new excited levels and over 100 new γ-ray transitions
- The 511-keV intensity (useful for diagnostics purposes) decreases by 15%
- As seen in PRC 102, 034316 (2020)

Measurement plan

- 135Xe + 135I proposal sent to ATLAS PAC 2021 (CARIBU beam)
- To maximize the impact of this project, we identified a series of radionuclides based on their importance in nuclear forensics, and on the poor quality of their nuclear data.

Lanthanum-140

- along with Ba-140, is a well-known chronometer used to date a nuclear event
- evaluated intensities originate from a single publication from 1991
- Production & Assay
  - Radioactive ^{140}La was produced at the UMass Lowell research reactor via (n,g) on ^{nat}La
  - The source was shipped to ANL for assay in Gammasphere (~ 3 days)
- La-140 Analysis, taken up by 3 SULI interns over the summer/fall: J. Ocheltree N. Cabanas N. Joseph
  - Consistent Matrix and Singles intensities - in most cases confirm the ENSDF intensities (1991CH05)
  - ~10 proposed new transitions
  - γ-γ angular correlation

Iodine-130

- "blocked" fragment, highly-sensitive to fuel/n-energy changes
- ENSDF based on a 1973 measurement, with more recent experiments reporting intensities disagreeing by as much as 10%
- Production & Assay
  - Purchase of enriched ^{130}Te and production of the irradiation target (J. Greene, ANL)
  - ^{130}I was produced at the BNL Tandem Van de Graaff via 7.5 MeV ^{130}Te(p,n)
  - The source was shipped to ANL for assay in Gammasphere (~ 1 day)

- S/N ratio improved by Compton suppression: 1000x more counts!
- Iodine-130 Analysis
    - 2 new levels
    - 23 new transitions
    - 3 re-placed transitions
    - T1/2 = 12.36(1) hrs
        - Evaluation dominated by < 1% uncertainty result
        - New preliminary value
    - Analyzed 27 γ-γ (ϑ) cascades

FY 2022 - planned measurements:

- I-135/Xe-135
    - ^{135}Xe has been identified for continuous monitoring for CTBT applications thanks to its low reactivity
    - ^{135}I yield remains nearly constant for all fission targets / energies (reference for other Iodine isotopes)
    - ^{135}Xe decay is based on one hand-written private communication from 1974
- Cerium-143
    - particulate fission product monitored as part of CTBT, and - along with other A=143 isotopes, important for predictions of inventory in used fuel assemblies
    - evaluated data originate from a single experiment performed in 1989
    - production through neutron irradiation of a sample of ^{nat}Ce at the UMass Lowell research reactor
    - αβγ decay station being commissioned at NNDC - BNL

This work could not have been done without Shaofei's help and expertise!

Recent Work related to Neutron Standards
11:10 - 11:25
Dr Allan Carlson

The Focus is on Possible Changes to the Neutron Standards Since the Last Standards Evaluation:

- Not all standards will be discussed – only relatively new data where important changes may occur
- Measurements will be discussed that will have an impact on the new evaluation of the Neutron Standards
- Possible changes in standards will be suggested but since the evaluation has not been done, final results can not be given

H(n,n)H Angular Distribution

- A very important measurement was done by Jiang et al.

    - Differential cross section data were obtained at 10 angles from 10 to 55 degrees. The measurements extend from 6 MeV to 52 MeV with 23 energy points. The flight path was 57.99m.
    - The measurements generally agree well compared with existing measurements, evaluations and theoretical calculations
- The hydrogen standard is limited to 20 MeV at the present time. The Jiang et al. data combined with the database being developed by Paris and Hale at LANL will allow an evaluation with an extended energy range to be produced. The present results are up to 50 MeV and Paris is hoping to have data up to 100 MeV by this CSEWG meeting.

H(n,n)H Angular Distribution Measurements by Jiang et al.

^{6}Li(n,t) Measurements

- Measurements have been made by Bai et al. that extend from 1 eV to 3 MeV with 80 energy groups and angular distribution measurements at each energy group for 15 angles between 19.2 and 160.8 degrees. Those data were normalized to the present standard in the interval from 0.1 to 0.4 MeV.
- The data may be overall the most complete, and best-quality, set of relative differential cross sections for the 6Li(n,t) reaction that presently exists at energies below 3 MeV.
    - The neutron energy spectrum was not measured at the position of the experiment. It is expected that this will affect the cross section values. It will not affect the angular distributions.
    - There are deviations from an isotropic angular distribution in the eV energy region. Some of this may be from problems due to the use of the 235U(n,f) cross section for determining the neutron fluence in regions where it is not smooth.
    - Also the integrated cross sections are below the standard for energies above 0.5 MeV, but within uncertainties. The magnitude of the cross section at the resonance peak differs from expected values. The agreement with the standard in many regions is relatively good. More work is planned.
- It is important to extend the energy range of this standard to above 1 MeV, the present limit of this standard. That would allow convenient overlap with H(n,n) standard. The Bai et al. data could possibly allow an energy range increase for this standard with more work on this experiment.

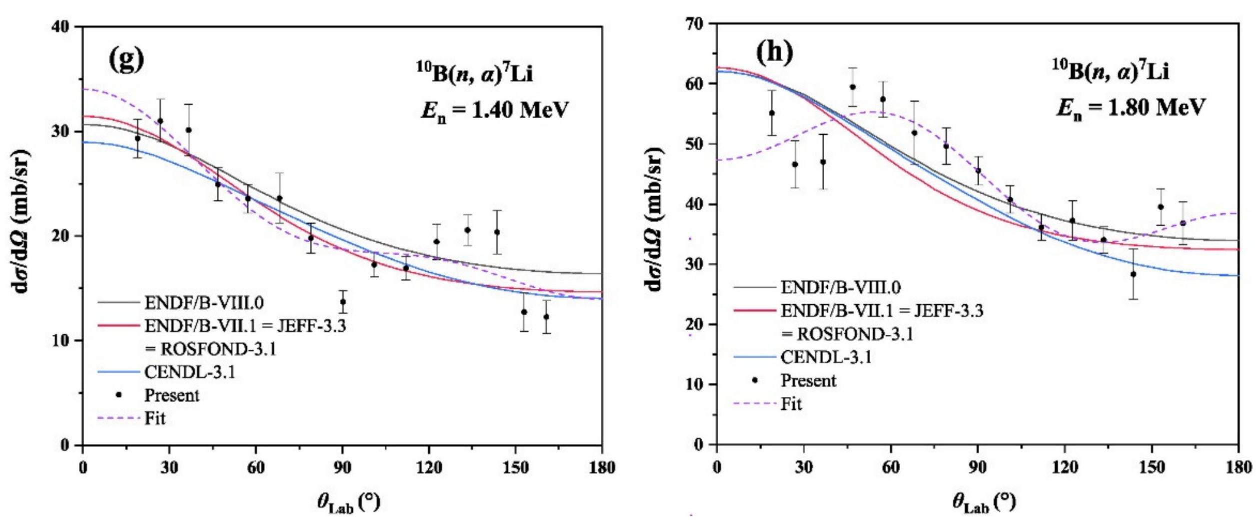
^{10}B(n,α) and 10B(n,α1γ) Measurements

- Several measurements of the10Be(p,n)10B reaction have been made by Massey and Jones-Aberty at Ohio University. The data include a measured excitation function at zero degrees and two selected angular distributions. Also a total neutron yield for the reaction was measured.
- Massey et al. have measured ^{10}B(n,Z) reactions for neutron energies from 2 to 20 MeV.
    - The work was done at the LANSCE WNR facility where proton, triton and alpha particles were measured at four angles. Differential cross sections were obtained for the 10B(n,p0)10Be, 10B(n,t0)8Be, 10B(n,a2)7Li and 10B(n,a3)7Li reactions.

The sum of the 10B(n,a0)7Li and 10B(n,a1)7Li differential cross section was measured. Partial angular distributions were obtained for the 10B(n,p1)10Be, 10B(n,t1)8Be and 10B(n,d0)9Be reactions.

- It has been submitted for publication.

- This wide range of data can all be used in R-matrix fits to improve the 10B standards since they all have the 11B compound nucleus.
- This cross section is now a standard only up to 1 MeV. These data should help in extending the energy of this standard to higher energies, possibly 3 MeV or higher.
- Work by Jiang et al. extends from 1 eV to 2.5 MeV with 59 energy groups. Data were obtained with at 15 angles between 19.2 and 160.8 degrees. These data were normalized to the present standard in the interval from 0.3 to 0.5 MeV. This is a very comprehensive complete set of measurements up to 2.5 MeV.
- The neutron energy spectrum was not measured at the position of the experiment. It will not affect the angular distributions.
- It was not possible to separate the a0 and a1 peaks for energies above 1 MeV. ¬ There are a number of cases where both the 10B(n,α1) and 10B(n,α) differential cross section data are somewhat low compared with the standard. The integrated 10B(n,α) cross section data are largely in good agreement but somewhat low in the several hundred keV energy region compared with the standard.
- The neutron fluence was the same for the Jiang boron measurements and the Bai lithium measurements. One experiment followed the other. Many problems in these experiments were remove by making them ratio data.
- A new experiment is planned where more precise appropriate spectrum measurement will be made. Also to improve separation of alpha peaks, a thinner sample and higher resolution detectors will be used then.
- These data in addition to those of Massey et al. should help in extending the energy of this standard to higher energies.



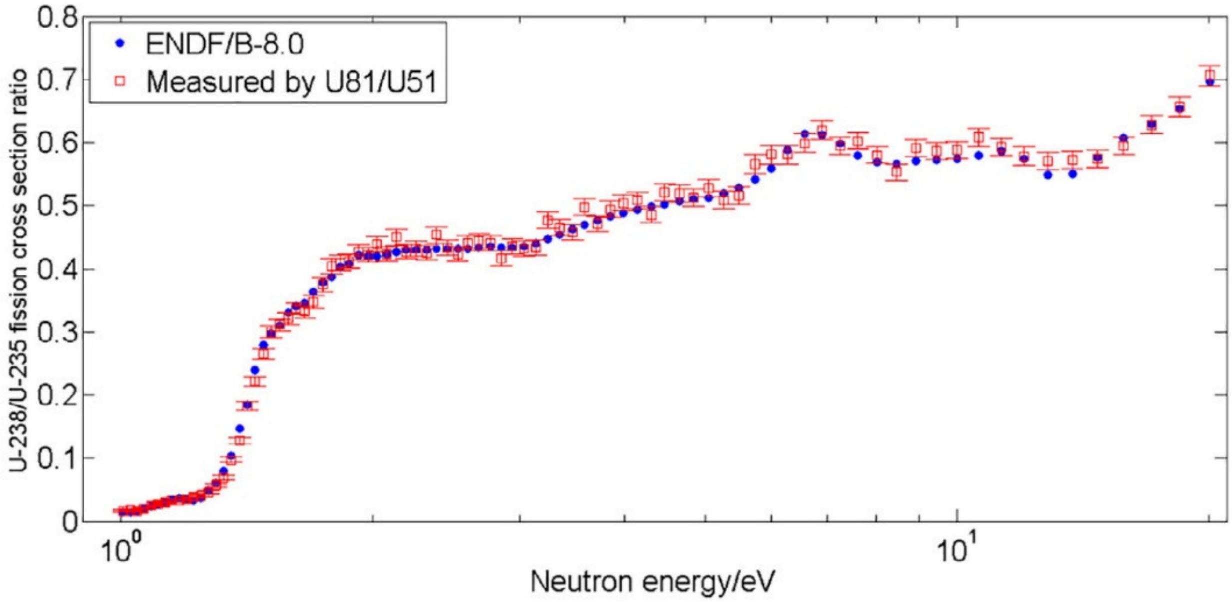
C(n,n) Cross Section

- The most recent evaluation of the carbon standard by Hale was done by combining 12C and 13C R-matrix evaluations to obtain the elemental cross section that is the standard. That evaluation, the ENDF/B-VIII standards evaluation (the 2017 standard), is somewhat higher than the ENDF/B-VII standards evaluation (the 2006 standard). The difference is most noticeable at the highest energies.
- Danon at RPI made total cross section measurements that are slightly lower than the 2017 standard values in the 150 to 400 keV energy region. Those data with uncertainties from a fraction of a percent to about 1% are in better than 1% agreement with the 2006 standards evaluation.
- Data at RPI also indicate differences with both evaluations at back angles (about 156 degrees) in the standards energy region.
- Hale is investigating this now

Fission Cross Section Measurements

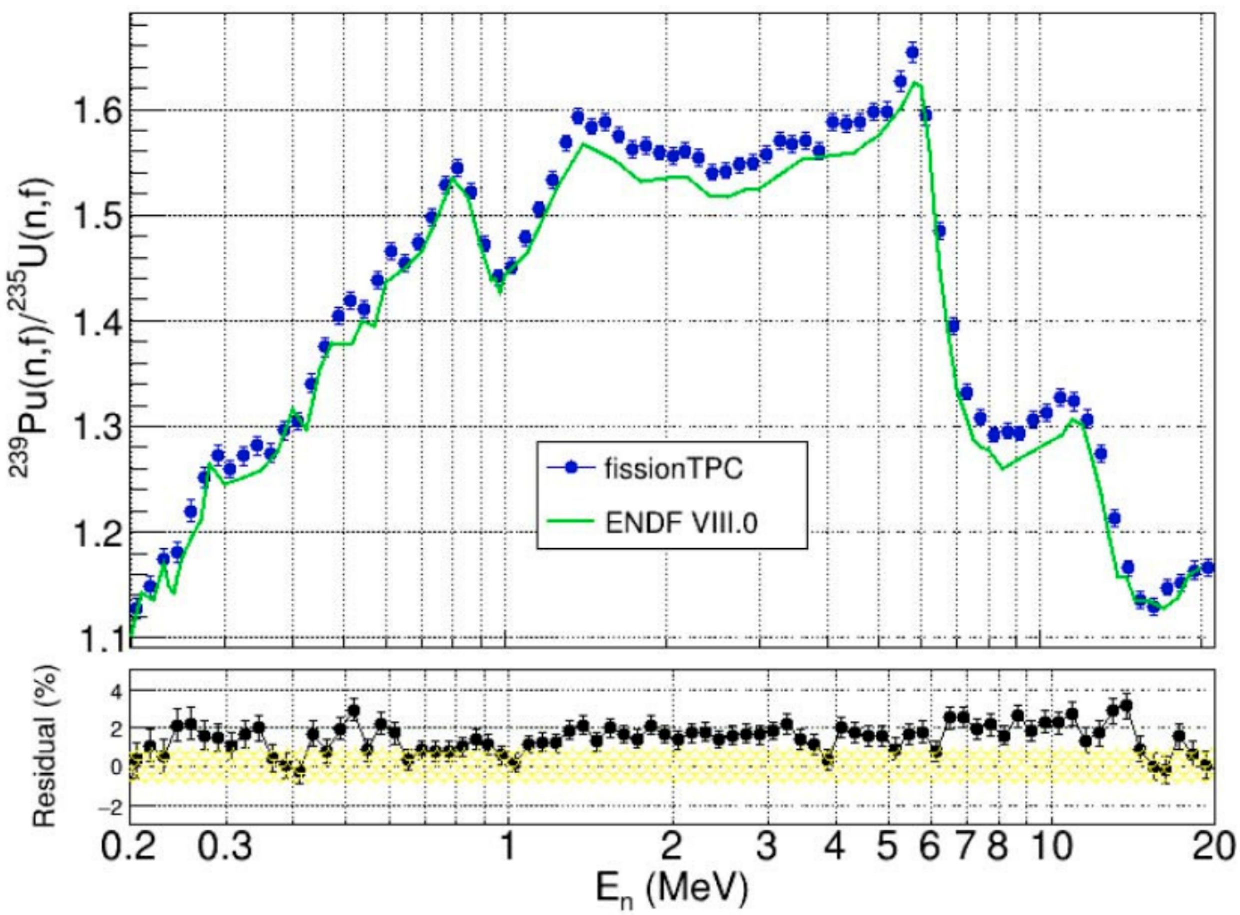
- Absolute measurements by the n_TOF collaboration were made of the 235U(n,f) cross section relative to hydrogen scattering from 10 MeV to 1 GeV. The analysis of the data from 10 MeV to 150 MeV is being done by Pirovano et al. The data analysis up to 1 GeV by Manna et al. is underway. The present standard is limited to 200 MeV. There is a strong need for an extension to higher neutron energies that may be possible with these data.
- Absolute measurements of the 238U(n,f)/ 235U(n,f) cross section ratio were made by Wen et al. up to 20 MeV. They agree with the standards results within their uncertainties of 2.3% to 3.6% .
- The Casperson et al., NIFFTE collaboration, measurements at LANSCE of the 238U(n,f)/235U(n,f) cross section ratio have been shown here previously. The data that extend to 30 MeV were normalized at 14.5 MeV to the present standards values. The agreement is quite good with the standard except in the region between about 2 and several MeV where their results are a percent or so low compared with the standard but generally within the uncertainties of the standard.
- 239Pu(n,f)/235U(n,f) cross section ratio measurements by Snyder et al. made at LANSCE by the NIFFTE collaboration have been submitted for publication. Those data are higher than the standards evaluation by about 2%. They agree in shape with the standards evaluation. New measurements are underway with an improved sample

238U(n,f)/ 235U(n,f) Cross Section Ratio Measurement at CSNS for One Cell Combination by Wen et al.



Denise asked if this data is ready to use. Allan said that he believes that the data is already published and therefore ready to be used.

Comparison of the NIFFTE 239Pu(n,f)/ 235U(n,f) Cross Section Ratio with the Standards Evaluation



Values almost constantly 2% higher than ENDF/B VIII.0

Use of Integral Data

- Starting with the standards for the ENDF/B-VI evaluation, very "clean" integral data were used.
- The data used were measurements of the 235U(n,f) and 239Pu(n,f) cross sections in the 252Cf spontaneous fission neutron spectrum (SACSs).
- Since there is a relatively small change in the cross section for these nuclides over most of the energy range of the 252Cf spectrum, an accurate determination of the cross section is possible. The result is also only weakly dependent on the uncertainty in the spectrum shape. These integral data basically help provide normalization for the standards evaluation.
- It was discovered that the spectrum averaged cross section values in our standards evaluation differed slightly from those in an IRDFF evaluation for the dosimetry community by Mannhart. This has led to an investigation of the two databases and concerns about some experiments due to insufficient documentation. Several other studies of inconsistencies are underway.
- This investigation is ongoing with no definite conclusions. Unfortunately, some data such as SACS ratios cannot be handled directly in GMA.

Additional Work that Impacts the Determination of the Standards

- Additional effort by Neudecker et al. on inspection of uncertainty sources for standards measurements
  - All data in the GMA database should be used and correlations should be taken into account for this investigation
- Further work on unrecognized sources of uncertainty
  - Inspection of data sets for unrecognized sources of uncertainty and correlations in data
  - Investigation of the energy dependence of USU for each standard
- Improved evaluation techniques for the standard cross sections
- The items above will be discussed at a virtual standards meeting on Dec. 6-10 in addition to:
  - Reviewing new experimental data
  - Discussing changes in the evaluation methodology and uncertainty quantification
  - Quantifying differences between new evaluations and the IAEA standards issued in 2017

Neutron and charged-particle cross section measurements
11:25 - 11:40
josh brown

The LBNL/UC-Berkeley Nuclear Data Program Experimental Activities

Experimental Activities

Fission Yields with FLUFFY:

- The Fast Loading User Facility for Fission Yields (FLUFFY) was developed at LBNL to rapidly shuttle actinide samples between a neutron source and counting array.
- Transport times: < 1s
- Flux: 8.3×10^8 n/cm^2/s
- This high flux along with the rapid transport time allows for the observation of 80+% of the yield in peak mass chains.

FIER Based Analysis

- The Fission Induced Electromagnetic Response (FIER) code offers a model that produces analogous FPY $\gamma\gamma$ emission data.
- Chi-squared minimization between FIER and experimental data is used to determine fission yields and correct decay data
- γ emission rates from the daughter FP simultaneously constrain the FPY and $I\gamma$ of the parent.

- An example of results from the A = 86 mass chain

TREND (Experimental Activities TRi-lab Effort in Nuclear Data)

- Targeted (p,x) stacked foil measurements for a variety of applications
- Development of a new analysis methodology for tuning model parameters in reaction codes
- Prompt-γ data collection being added to upcoming experiments
- How do we improve modeling for high-energy proton-induced reactions?

R&D Supporting DoE Isotope Production

- 236Np Production R&D
    - Performed 3 target stack irradiations and γ-spec at LBNL
    - ICP-MS & α-spec at LANL
    - 16 MeV: 56.8(9) ng/mA•hr, 28 MeV: ≈200 ng/mA•hr
    - 12 targets (99.94% 235U) made by LLNL with ρR_{areal} from 80-160 μg/cm2
    - We could meet the demand of 10-20 μg/yr 236Np in a short time at Id >100 μA.
- Novel Methods for Producing 229Th
    - New methods for production of 225Ac have been identified

(n,n’γ) with GENESIS

GENESIS Array Characterization

- Absolute efficiencies established using a combination of gamma ray and neutron sources
- Long dwell time 252Cf measurements enabling model tuning, detection efficiency calculations, and time calibrations
- Three experiments conducted in 2021:
    - 238U March
    - 56Fe July
    - 35Cl Aug
- GENESIS+ for Cl Measurements
    - Additionally targeting (n,p) and (n,α) during Cl measurement
    - Inclusion of an active target CLYC for σ (En)
    - NaCl salt co-located with Ni foil to provide integral σ for the experiment

Neutron response of organic scintillators

- Scattering experiment using active “target” scintillator
- Map light vs nuclear recoil energy (highly non-linear)
- Kinematically over- constrained system allowing rejection of multiple scatters
- Continuous measurement using broad energy neutron source
- Neutrino detection (background identification in IBD detectors see WoNDRAM report) WbLS, Gd doped WbLS, Li-loaded plastics
- Nuclear security & non-proliferation (kinematic reconstruction for imaging) Commercial fast plastic scintillators (EJ-20X, EJ23X) and custom organic glass

- Nuclear physics experiments(threshold estimation and forward modeling approach) Commercial PSD liquids (EJ-301, EJ-309)
- Nuclear fusion (diagnostics of plasma instabilities for Z-Pinch device) Commercial fast plastics(EJ-204)

13C(α,n)16O studies at the University of Notre Dame
11:40 - 11:55
James deBoer

Motivations

- Large mass detectors for neutrino and dark matter detection (e.g. CDMS, DUNE, KamLAND)
    - Actinides and light elements (carbon, oxygen, etc.) are hard to completely remove from setups
    - Actinide decays -> up to 9 MeV α-particles -> (α,n) on light nuclei in the environment
- Neutron applications
    - Sources4c modernization
    - ^{19}F, ^{18}O, ^{17}O, $^{13}C(\alpha,n)$ reactions
    - For example, data evaluation of the ^{17}O system, $^{16}O(n,\alpha 0)^{13}C$ (See Mark Paris' talk on Wednesday at 15:20 and Thursday at 13:55 EST.)
- Nuclear Astrophysics
    - (main) s-process neutron source: $^{13}C(\alpha,n)^{16}O$, $^{22}Ne(\alpha,n)^{25}Mg$, $^{17}O(\alpha,n)^{20}Ne$, $^{18}O(\alpha,n)^{21}Ne$, $^{25}Mg(\alpha,n)^{28}Si$, $^{26}Mg(\alpha,n)^{29}Si$
    - First stars: 10,11B(α,n)13,14N
    - 100 keV to a few MeV
- See (Paraskevi) Vivian Dimitriou's talk on Wednesday at 15:40 EST

One way we can improve (α,n) type reactions: Angular distribution, partial cross section measurements working hand in hand with high statistics 4π counter measurements.

Level diagram of ^{17}O system

- Lots of levels!
- First excited state is 0^+: De-excites via pair production
- 2nd, 3rd, and 4th excited states decay through γ-ray emission with nearly 100% probability to the ground state

Enough levels to complicate R-matrix but not enough to go to Hauser-Feshbach.

Nuclear Science Laboratory (NSL) at the University of Notre Dame:

- isnap.nd.edu

- 5 MV single ended accelerator
    - dc alpha beam, alphas from 300 keV up to 9 MeV
    - up to 100 uA of beam on target
    - Usually using 10 uA for these studies
    - Energy resolution of better than 1 keV, energy uncertainty of less than 10 keV

Dec 2020 setup, ND 5U "solid target" line developed by Michael Febbraro (ORNL)

New measurements (Dec 2020)
υ 13C(α,nγ) using GEANIE HPGe @ 45 degrees υ First measurements of 13C(α,αγ)13C υ Could separate 6.92 and 7.12 MeV transitions with HPGe

13C(α,n0) angular distributions from ODeSA measurements

- About 20 keV energy steps
- 20 point angular distributions
- Uncertainties are usually about 5% (unfolding dominated)
- Measurements actually go up to 9 MeV, but our current measured detector response only allows us to go up to 6.5 MeV

13C(α,n1) measurements, Feb 2021
• Michael Wiescher • ND 5U accelerator • DC alpha beam • 10 ug/cm2 13C target (György Gyürky) • 30 uA on target • 30 minute runs • Typically a few hundred counts

First measurement of 13C(α,n1) cross section (plus MCMC analysis)

Comparison with evaluations (Marco Pigni did the SAMMY calculations of Heil's R-matrix fit)

Improvement in uncertainty analysis

- Development of a Bayesian uncertainty analysis routine for the AZURE2 R-matrix code has been ongoing
- Daniel Odell, a postdoc at OU, is the main developer
- This work is possible thanks to Daniel Phillips and Carl Brune and a grant from NNSA

Showed plots of the fit parameter covariance matrix. Will be included in upcoming PRC article

Summary and Foreword

- We've measured 13C(α,n0), 13C(α,n2γ), 13C(α,n 3 γ), and 13C(α,n 4 γ) in the higher energy range (5 to 9 MeV) and 13C(α,n 1) from 5 to 6 MeV
- Future work
    - Measure detailed angular distributions of 13C(α,n 0) from about 1 to 5 MeV (in two weeks)

- Measure ODeSA response matrix up to 20 MeV at LANSCE (done last week!)
- Expand (α,n 1) measurements from 6 to 9 MeV

The present status of the EXFOR project
11:55 - 12:10
Dr Boris Pritychenko

Nuclear Reaction Data Compilations in USA & Worldwide

- Experimental neutron reaction data compilations have been pioneered at the Metallurgical Laboratory, University of Chicago and Los Alamos National Laboratory in 1945-1947.
- Brookhaven National Laboratory hired many Manhattan Project alumni when it was founded in 1947, and the lab got involved in nuclear data.
- Donald J. Hughes (1915-1960) was behind the BNL-170 (1952); it is a precursor of BNL-325 (Atlas of Neutron Resonances).
- SCISRS (Sigma Center Information and Retrieval System) at BNL (1964) was a precursor of EXFOR.
- Other data centers were created in Paris, France (NEADatabank), Vienna, Austria (NDS-IAEA), and Obninsk, USSR (IPPE) in 1963-1964.
- Around 1970 four neutron data centers agreed on the data interchange format (EXFOR). The four centers could store data locally in its formats. The Nuclear Data Centres Reaction (NRDC) network was founded in 1979 under the auspices of the IAEA.

EXFOR - Experimental Nuclear Reaction Data

- The largest experimental nuclear reaction database (www.nndc.bnl.gov/exfor)
  - 23,889 experiments (multiple publications are grouped into a single measurement).
  - 177,449 data sets as of October 1, 2021.
  - Essential for Evaluated Nuclear Data File (ENDF) libraries worldwide.
  - Presently run by the Nuclear Reaction Data Centres (NRDC) internationally. This is an IAEA network which is coordinated by the IAEA.
  - Two largest contributors: NNDC & NEA-Databank.
  - Every second, third and sixth data points in the library were contributed by the NNDC, NEA-Databank and the rest of NRDC network, respectively.

EXFOR philosophy is to compile data as they were published (in consultation with authors) unless obvious errors are found. Published nuclear reaction data contain outliers and discrepancies.

Area #1 FY 2021 Statistics

- New compilations: 131
- Updated compilations: 303
- Finished compilations of missing fission yields, NRDC memos: CP/C-0464, CP/C-0465, CP/C-0466, and CP/D-979.
- Preliminary NRDC transmissions: 26
- Final NRDC transmissions: 17
- EXFOR DB Updates: 40
- EXFOR Web retrievals
  - CINDA: 1,479
  - ENDF: 101,045
  - EXFOR: 44,387

Working Party on International Nuclear Data Evaluation Co-operation (WPEC) – SubGroup 50

Subgroup on developing an automatically readable, comprehensive and curated experimental reaction database (LA-UR-20-22620).

US Nuclear Data Program EXFOR modernization effort

- Create a parallel library to EXFOR that stores and incorporate corrections to data and uncertainties that were undertaken by evaluators. Also, store expert judgment on these data.
- Assess published uncertainties with templates of expected uncertainties for specific measurement types.
- Use artificial-intelligence and machine-learning algorithms in conjunction with comprehensive physics models for outlier identification.

USNDP EXFOR Modernization Proposal

- Work on SubGroup50 requires funding.
- We propose to re-analyze the EXFOR database contents, develop corrections for many data sets, flag discrepancies, introduce covariances, and store the high-quality curated data in a parallel (sister) database.
- We will employ artificial-intelligence and machine learning (AI/ML) algorithms, re-visit nuclear reaction monitor and decay data values in conjunction with comprehensive physics models in order to enable outlier identifications in data selection.
- We will also translate the data in EXFOR from the historic exchange to JavaScript Object Notation (JSON) format and develop an application programming interface (API) to facilitate code interfacing and provide a pipeline between experimentalists, compilers and evaluators.

Database Integration:

- ENSDF/XUNDL/NSR databases are integrated.
- 59,093 out of 240,594 NSR references are used in ENSDF.
- Recently, in collaboration with the NDS-IAEA (V. Zerkin), we integrated NSR and EXFOR.
- How many EXFOR compilations are used in ENDF???
- It could be nice to include relevant EXFOR accession numbers into ENDF evaluations and build better connections with the EXFOR project.
- Eventually, it would help to create a single nuclear data library.

Takeaways

- NNDC EXFOR compilation efforts are complex and well-organized: B. Pritychenko (BNL), O. Schwerer, S. Hlavac, O. Gritzay (Under contract with BNL), V. Zerkin (IAEA).
- SG50 & USNDP EXFOR Modernization project.
- 75th anniversary of nuclear reaction data compilations in 2021-2022.

Q Roberto: SG 50 is modernization of EXFOR or complementary (parallel library/interface)?
A Denise: Yes, we are not trying to replace EXFOR, but rather an effort to bridge EXFOR to evaluators.
A Boris: EXFOR will

Session: Validation Committee

Introduction
13:10 - 13:15
Dr Michael Zerkle

Welcome to the Validation Committee Session

ENDF Phase 1 Checking & Review Status
13:15 - 13:30
Dr Dave Brown

Phase I checking

ADVANCE status

Current ADVANCE system has several shortcomings:

- Uses buildbot “substrate”. Gitlab doesn’t like buildbot. Gitlab likes Kubernetes

- ADVANCE watches only one branch
- ADVANCE checks whole library and each evaluation, but only reports on the whole library

ACTIONS:

- Get Kubernetes cluster running
- Divorce ADVANCE from buildbot (right now is more of a separation than a divorce…) (DONE)
- Kill all the bugs being introduced during the divorce process
- Allow ADVANCE to watch all branches
- ADVANCE should check whole library only for phase2 & master branches
- ADVANCE should check each evaluation only and provide report as build artifact to gitlab

ENDF branches & review process

ENDF project branches & workflow presented

Action items:

- Describe review process in CONTRIBUTING.md files
- Review forms for all sub libraries (you all agreed for now they can be the same)
- Gather comments for review forms
- Code to generate a phase2 merge request with new branch holding new evaluation
- Code to generate reviewer form,
    - Used legacy forms as starting point
    - Template generates Markdown form that plays nice with gitlab
    - Add link to prior phase1 evaluation
    - Connect review form to MR automatically
- Set up reviewer notifications in gitlab
- Reviewers for all sub libraries - we have some names, but not for all sub libraries and not all reviewers have gitlab accounts

We can and will start reviews. It will be rough until we iron out remainder of technical issues

Dave did a live demonstration at the GitLab website.

Andrew Holcomb suggested merging to Phase 2 using cherry-picking merge to preserve history. Dave considered studying that an action item.

Mark Paris said that he could re-submit the Li evaluation, since he has done many changes since it was submitted still in GForge.

Dave: Cyber security requires that GitLab can't tell ADVANCE to do something. ADVANCE has to ask GitLab things and decided on its own what to do. Transition to Kubernets should help in this process.

Andrew Holcomb said that they now in ORNL have a lot of experience with Git and offered to help. However, they have two GitLabs, one outward and one inward. While BNL has only one Git repository outside the firewall while ADVANCE sits inside.

Mike Herman asked about how to add additional materials. No simple solution.

ORNL Experience with the ENDF/B-VIII.0 Graphite TSL Evaluations
13:30 - 13:45
Friederike Bostelmann

Introduction

- Up to the ENDF/B-VII.1 release, the graphite TSL evaluation always assumed 0% porosity (perfect graphite crystal)
- ENDF/B-VIII.0 provides graphite TSL evaluations for 0%, 10% and 30% porosity
- The ENDF/B-VIII.0 data was processed with AMPX into continuous-energy (CE) and multigroup (MG) libraries for use in SCALE (to be released with SCALE 6.3.0)
- The impact of the choice of the graphite TSL evaluation was assessed using three benchmarks from the International Handbook of Reactor Physics Experiments

Tools

- Neutron transport using SCALE 6.3 beta:
    - KENO-VI Monte Carlo
    - Shift Monte Carlo
- Nuclear data libraries:
    - Continuous-energy library
    - 252-group cross section library
    - ENDF/B-VIII.0 data:
        - 0% porosity: "graphite"
        - 10% porosity: "c-10_graph"
        - 30% porosity: "c-30_graph"
        - No TSL data: "carbon"

Model 1: HTR-10

- 10 MWth Pebble-bed High Temperature Gas-cooled Reactor
- Relevant characteristics:

- UO2 fuel density: 10.4 g/cm3
    - 235U enrichment: 17 wt.%
    - TRISO packing fraction: ~9%
    - Number of particles per pebble: 8,385
    - Pebble radius: 3 cm (fuel zone: 2.5 cm)
    - Graphite densities indicate porosities between 19–30%
        - Dummy pebbles: 18.6%
        - Fuel pebbles (matrix, shell): 23.5%
        - Reflector and carbon brick: up to 30%
- HTR-10 initial criticality:
    - 9,627 fuel pebbles
    - 7,263 dummy pebbles
    - 61% packing fraction
    - Room temperature
    - Fresh fuel

Model 2: HTTR

- 30 MWth Prismatic High Temperature Gas-cooled Reactor
- Relevant characteristics:
    - UO2 fuel density: 10.39 g/cm3
    - 235U enrichment: 3.4–9.9 wt.%
    - TRISO packing fraction: 30%
    - Number of particles per fuel compact: 12,987
    - Fuel compact inner radius/outer radius/length: 1 cm/2.3 cm/3.9 cm
    - Graphite densities indicate porosities between 22–25%
        - Graphite overcoat and cladding: 24.8%
        - Graphite reflector around blocks: 24.0%
        - Graphite in blocks: 22.2%
- HTTR criticality experiment:
    - Configuration with fully loaded core (30 fuel blocks)
    - Room temperature
    - Fresh fuel

Model 3: MSRE

- Molten Salt Reactor Experiment
- Relevant characteristics:
    - Salt is a mixture of:
        - the carrier salt containing the beryllium, zirconium, and most of the lithium fluorides,
        - depleted uranium eutectic (73LiF-27UF4), and
        - highly enriched uranium eutectic (73LiF-27UF4).
    - Graphite stringer height: 170.31 cm
    - Graphite stringer pitch: ~5.08 cm

- Graphite density indicates porosity of 18.12%
- MSRE initial criticality:
  - Besides shield and insulation, all materials at 911 K
  - Fresh fuel

International Handbook of Reactor Physics Experiments," Molten-Salt Reactor Experiment (MSRE) zero-power first critical experiment with U-235" MSRE-MSR-EXP-001, OECD/NEA, 2019.

Impact of graphite TSL evaluation on the HTR-10

- The fuel temperature was increased to 1,200 K, and all other temperatures were increased to 1,000 K.
- Large impact at cold temperatures
- Major impact for graphite in fuel pebbles

Impact of graphite TSL evaluation on the HTTR

- The fuel temperature was increased to 1,200 K, and all other temperatures were increased to 1,000 K.
- Large impact at room temperature
- Major impact for graphite in compact

Impact of graphite TSL evaluation on the MSRE

- Large impact at room temperature

Comparison with benchmark results

- HTR-10 and HTTR: Best agreement with benchmark results when using 0% porosity.
- MSRE: Large difference to benchmark caused by e.g. uncertainties in the fuel composition
  - No conclusion with regard to the choice of graphite TSL evaluation is drawn.

Conclusions

- Impact of the choice of graphite TSL data on the eigenvalue of the HTR-10, HTTR, and MSRE:
  - Observed only for low temperatures
  - Largest impact observed for TRISO-fueled HTGRs
  - Largest impact in HTGRs observed for graphite in fuel components (pebble, compact)
  - Best agreement with benchmark eigenvalue observed with 0% porosity
- Additional considerations:
  - Information about graphite porosity is not provided in the benchmark specifications of any of the studied models
  - Porosity could be estimated based on theoretical graphite density
  - Graphite porosity changes as a function of neutron fluence

Validating the LANL versus INDEN 239Pu file in the fast range
13:45 - 14:00
Dr Denise Neudecker

239Pu files validated:

- ENDF/B-VIII.0
- LANL file:
  - New fission source term: PFNS (Chi-Nu+CEA data, INDEN at thermal), nu-bar (Marini data, CGMF modeling), (n,f) cross section (updates according to template, fissionTPC),
  - New (n,g) cross section (closer to Mosby, M1 enhancement),
  - New scattering data (Engelbrecht-Weidenmuller, removal of fictitious levels).
- INDEN files: Empire p27, ORNL/IAEA/JSI RR parameters, VIII.0 (n,g), fission source term from LANL file,
  - p29: + IAEA nubar + Empire (n,2n),
  - p35: + LANL nubar + Empire (n,2n),
  - p38: + LANL nubar + VIII.0 (n,2n).

keff of PMFs and PMIs with INDEN files: all 3 perform well.
Mean bias:

- p29: 104 pcm
- p35: 98 pcm
- p38: 98 pcm
- VIII.0: 78 pcm

keff of PMFs and PMIs with LANL files: small tweak needed.
Mean bias:

- 11/1: 130 pcm
- 11/1ps: 129 pcm
- VIII.0: 78 pcm

Benchmarking of reaction rates in Jezebel critical assembly. INDEN and LANL are reasonably close to VIII.0.

Pulsed spheres various INDEN files: virtually the same and all good.
Pulsed spheres VIII.0 vs LANL -> Under active development!

LANL is currently working on tweaking for better prediction of pulsed spheres.

We gratefully acknowledge the support of the Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory.

Current status:
- INDEN performs well on keff, pulsed spheres and many RR (Pu9(n,g)/(n,f) needs some work),
- LANL performs reasonably well on keff and RR, some work on pulsed spheres needed.

Q Andrej: Where do you take the models and uncertainties from?
A: Forwarded propagate uncertainties to account for experimental and Monte Carlo uncertainties. Models taken from Skip Kahler's input decks.

The impact of FENDL-3.2 on ITER and FNSF fusion reactor computational benchmarks
14:00 - 14:15
Tim Bohm

Same as before but now we have a new version of FENDL, released earlier this year.

Outline
1) Introduction
2) Nuclear data libraries examined
3) Benchmark/Systems Analyzed:
- ITER-1D computational benchmark
- FNSF-1D computational benchmark

4) Future Work

Current D-T Fusion Experiments/Reactors
- JET (UK)
  - 1983-present
  - Rmajor=3 m
  - Vol_{plasma}=100 m3
  - pulse ~1 sec
  - 16 MWfusion
- ITER (France)
  - under construction
  - R_{major}=6 m
  - Vol_{plasma}=840 m3
  - pulse ~400-600 sec
  - 500 MWfusion D + T -> He-4 (3.5 MeV) + n (14.1 MeV)
- Soon, maybe? private start-ups (not all D-T or Tokamak based)
  - Helion, Common Wealth Fusion, General Fusion, TAE Technologies
  - Several others

Important Fusion Neutronics Responses

- Neutron flux/fluence
    - structure, magnets
- Total nuclear heating (neutron+photon)
    - coolant system design, thermal stress, etc. for structure, magnets
- Tritium production (neutron)
    - breeding fuel, environmental concerns
- Radiation damage/dpa (neutron)
    - structural material, magnet degradation
- Helium production (neutron)
    - re-weldability
- Radiation dose (neutron+photon)
    - insulators, electronics, personnel
- Activation
    - shutdown dose-maintenance robotics, personnel
    - decay heat-safety (LOCA, LOFA)
    - radioactive waste disposal, recycling

Nuclear heating in ITER FW/Shield Block Tritium production in FNSF breeding channel

FENDL Library

- The Fusion Evaluated Nuclear Data Library (FENDL) is an international effort coordinated by the IAEA Nuclear Data Section
- Assembles a collection of the best nuclear data from national cross section data libraries for fusion applications
    - ENDF/B (US), JENDL (Japan), JEFF (Europe), TENDL (EU), RUSFOND/BROND (Russia)
- Process uses fusion specific experimental and calculational benchmarks to evaluate the data
- Data available on-line

Source of FENDL Data

- 65/180 isotopes in FENDL-3 come from ENDF/B-VII.1
    - See Table 1 in INDC(NDS)-0628
- Some key isotopes for this work are H-1, O-16, Cr-52, Fe-56, Ni-58, Cu-63,65

Goal of this work

- Look at the neutronics impact of using the updated neutron libraries in a realistic model of fusion systems using MCNP
- Libraries examined:
    - Neutron:
        - FENDL-2.1 (21c)
        - FENDL-3.1 (31c)-current version 3.1d

        - Initial INDEN evaluations for O, Cr, Fe*
        - FENDL-3.2 (32c)-june 24, 2021 version
            - Includes newer INDEN evaluations for O, Cr, Fe
        - ENDF/B-VII.1 (80c)
        - ENDF/B-VIII.0 (00c)
    - Photon:
        - mcplib84 (84p)**
- Previous work has shown that mcplib84 produces results similar to the newer MCNP eprdata12 library, the latest MCNP photon library (eprdata14) has not been tested yet

* Bohm T.D, Sawan M.E. "Neutronics calculations to support the Fusion Evaluated Nuclear Data Library (FENDL)", Fusion Science and Technology, on-line early access August 2021.
**Bohm T.D, Sawan M.E. "The impact of updated cross section libraries on ITER neutronics calculations", Fusion Science and Technology, Vol 68, p. 331-335, 2015.

ITER 1-D Cylindrical Calculation Benchmark

- Based on an early ITER design
- Developed for the FENDL evaluation process
- Simple but realistic model of ITER with the Inboard and Outboard portions modeled with the plasma in between
- D-T fusion (14.1 MeV neutrons)
- Flux (neutron and photon), heating, dpa, and gas production calculated
- M. Sawan, FENDL Neutronics Benchmark: Specifications for the calculational and shielding benchmark, INDC(NDS)-316, December 1994

Results: Neutron Flux ITER

- ENDF/B-VIII.0+CrInitial, FeInitial closer to FENDL-2.1 but see structure at VV, TF Coil
    - main difference due to Ni and Cu XS respectively
- FENDL-3.1+CrInitial, FeInitial quite close to FENDL-2.1 but structure at VV (Ni)
- FENDL-3.2 even closer to FENDL-2.1

Results: Total Nuclear Heating ITER

- FENDL-3.2 see peak at H2O regions and TF coil insulator (low Z) • neutron heating up to 4X>photon heating in water regions

Neutron Heating Numbers in Water

- Neutron fluxes similar in water regions
- Neutron heating numbers in water are similar except at very low and very high energies (8-15 MeV)
- Using FENDL-2.1 for transport and heating tallies with variety of XS libs indicates that different heating numbers are the cause for the FENDL-3.2 heating differences in water

1-D FNSF Cylindrical Computational Benchmark

- Next generation will be very different than ITER
- Need to test XS libraries on fusion designs other than ITER (different structural materials, coolants)
- Created 1-D model of Fusion Energy Systems Studies Fusion Nuclear Science Facility (FESS-FNSF)
- Breeding Zone: He cooled steel structure (90 w/o Fe, 7.5w/o Cr, 2w/o W, 0.2w/o V), PbLi breeder
- 85 radial zones
- Includes SiC flow channel inserts in breeding zone
- Includes face plates and filler for SR, VV, Ltshield
- Includes IB, OB magnet and cryostat
- MCNP materials created with PyNE
- T. Bohm et al. "Initial Neutronics Investigation of a Liquid Metal Plasma Facing Fusion Nuclear Science Facility, Fusion Science and Technology, 2019.

Results: Neutron Flux FNSF

- All libs show higher flux than FENDL-2.1 (except FENDL-3.2 at OB CC, WP)
- FENDL-3.1d shows highest flux (also seen in ITER benchmark)
- ENDF/B-VIII.0 & FENDL-3.2 quite close up to depth of IB LTshield and OB VV
- FENDL-3.2 vs FENDL-3.1d flux values 6% lower at IB CC, 15% lower at OB CC

Results: Total Nuclear Heating FNSF

- Heating in tungsten at FW is lower for FENDL-3.2 and 3.1d compared to FENDL-2.1
- All libs show higher heating than FENDL-2.1 beyond the Breeder except FENDL-3.2 at OB WP (not seen in the ITER benchmark)
- All newer libs show some significant differences esp. at deep locations (LT, CC,WP)
- FENDL-3.2 peaks are in BZ channel walls, BW, OB SR back plate (MF82H)

Results-Tritium Breeding Ratio FNSF

- FNSF uses PbLi for breeding:
    - 84.3 atomic% Pb
    - 15.7 atomic% Li (enriched to 90% Li-6)
- Recall 1-D model includes He cooled flow channels for the PbLi with thin SiC inserts
- TBR ~1.2-1.8% higher than that calculated with FENDL-2.1
- Newer libraries are quite close to each other

Future Work:

- Plot dpa, He production, T production results (for both benchmark models)
    - already calculated but not plotted and studied in detail
- Dig into differences of heating in FNSF model
- Add more resolution for heating tallies

Discussion:

Water heating (peaks seen in heating) is concerning. Roberto suggests that this is due to VIII.0 oxygen. Andrej suggests to adopt oxygen from JENDL.

Validating Gamma-rays Produced in Nuclear Reactions
Isabel Hernandez

There are many applications using neutron-induced gamma signatures at LLNL:

- Exploration (earth, planetary)
- Verification (warhead monitoring)
- Identification (emergency response)

Goal: Validate nuclear models for inelastic scatter

- Simulations require validated nuclear data libraries
- Investigate differences between experiment and simulation
  - Measurement vs. Evaluation
  - Evaluation vs. Simulation

Measurement vs Evaluation: Challenges with non-discrete data

- Examined gammas produced from 14.5 MeV inelastic scatter with neutrons on common isotopes
  - Compared values in data libraries to experimental compilation from IAEA
  - Used FUDGE to extract data from ENDFB-VIII.0 in GNDS
  - Discrete (MT 51-90) and non-discrete (MT 91) data
  - Correct interpretation of non-discrete data was unclear

Discrete and Continuum Contributions are Stored Differently in Libraries

Non-discrete contributions are needed to match experimental data

- Explored different integral windows for non-discrete spectrum
- For 14 MeV neutrons, non-discrete contributions are needed to match the experimental data (INDC/IAEA)

Measurements vs. Evaluation: Some issues also observed with discrete data

- ^{16}O Spectrum
  - Unique discrete spectrum
    - Histogram-like storage
    - E_γ = 0.97, 1.75, 1.95 MeV not accounted for
- ^{14}N Spectrum

  - No gamma-ray production FUDGE files for inelastic excitation states
    - All inelastic data associated with MT=4
    - Cross sections of MT=51-91 matches MT=4

Transport codes also interpreted data differently

- Examined how Monte Carlo radiation transport codes interpret data
  - MCNP, Mercury, GEANT4 with ENDFB-VIII.0
  - Broomstick geometry to tally reactions
  - Ratio of (inelastic/total) neutron reactions
- Large differences observed for some isotopes: analysis of ^{12}C and ^{14}N are key to non-destructive techniques for cargo screening

Discussions with data teams suggests improvements for evaluations

- Examined the energy binning structure for gamma decays following inelastic scatter
- Too few bins suggests unphysical spectra

Examined inelastic data: room for improvement

- Issues identified for gamma-rays produced with 14 MeV neutrons, particularly for non-discrete data
- Encourage further attention to these data - scatter reactions are important for many applications, and accurate data are needed

References:

1. Simakov, S.P., Pavlik, A., Vonach, H., & Hlavac, S. (1998). Status of experimental and evaluated discrete γ-ray production at E_n=145 MeV Final report of Research Contract 7809/RB, performed under the CRP on measurement, calculation and evaluation of photon production data (INDC(CCP)--413). International Atomic Energy Agency (IAEA)
2. Castaneda, C., Gearhart, D., Gearhart, R., Sanii, B., Englert, P., Dempsey, J., Young, J., Drake, D., & Reedy, R. (2007). Gamma ray production cross sections from the bombardment of Mg, Al, Si, Ca and Fe with medium energy neutrons. *Nuclear Instruments & Methods in Physics Research Section B-beam Interactions With Materials and Atoms, 260*, 508-512.
3. El Kanawati, W., Perot, B., Carasco, C., Eleon, C., Valkovic, V., Sudac, D., Obhodas, J., & Sannie, G. (2011). Acquisition of prompt gamma-ray spectra induced by 14 MeV neutrons and comparison with Monte Carlo simulations. Applied radiation and isotopes : including data, instrumentation and methods for use in agriculture, industry and medicine, 69(5), 732–743. https://doi.org/10.1016/j.apradiso.2011.01.010

Session: ND 2022 Announcements

ND 2022 status update

15:20 - 15:35
Caleb Mattoon

ND2022 to be held July 24-29, 2022. We are planning for an in-person event, but preparing for virtual or hybrid just in case…

- Over 450 abstracts submitted
- Most attendees indicate interest in attending in-person, but uncertainty due to Covid19 could still force the event to switch to remote
- Please fill out the registration survey if you haven't already: https://indico.bnl.gov/event/9462/registrations/449/
- Conference has been registered with U.S. Department of State § Some conference logistics still very much in flux…

In-person event planned for July 24 – 29, 2022 at the SAFE Convention Center in Sacramento, CA

Venue: SAFE Credit Union Convention Center (recently remodeled)

Key dates:

- Website + abstract submission went live July, 2021
- Abstract submission deadline extended to October 20, 2021
- Speakers / poster presenters notified December 2021 (deadline may slip to January)
- March / April 2022, estimated deadline to reserve hotel rooms
- ND2022: July 24 – 29, 2022
- August – October 2022 accepting proceedings papers
- Fall 2022 - Summer 2023 complete refereeing process and publish proceedings
    - Proceedings to be published online-only with EPJ Web of Conferences

Abstract submission closed in mid-October, abstract review getting started

- 478 abstracts submitted by 415 authors
- Assuming 6 parallel sessions over 4 days, we have time for around 400 standard / invited talks
    - Likely need a shorter 'flash talks' session as well as poster session
- Some authors already indicated that they can only participate remotely

Other logistics

- Keynote addresses partly finalized
    - LLNL director Kim Budil to provide opening address
    - DOE representatives to discuss outstanding nuclear data needs

    - Reviews of recent improvements in theory, experimental capabilities, evaluated data libraries, applications
- Working on bringing students to present their research and help with conference logistics
    - Thanks to ANL, LANL and LBNL for offering student support!
- Planning to hold a banquet at the Sheraton.
- Still working to attract sponsors!

Hotel room blocks are still being worked out…

- We initially planned for 400 rooms at federal per diem ($145/night). Those negotiations were put on hold in early 2020 due to Covid. We have resumed negotiating, but for a smaller room block.
- Hotels nearest the convention center are asking for higher attrition / cancellation rates than LLNL is willing to sign. We're looking at other nearby hotels with some success — One hotel offered 0 attrition but was then sold and will no longer be a hotel next year!
- We are still working on expanding available rooms but may not be able to offer enough rooms at per diem for all attendees!

Options for hybrid event (or in case we need to switch to fully remote)

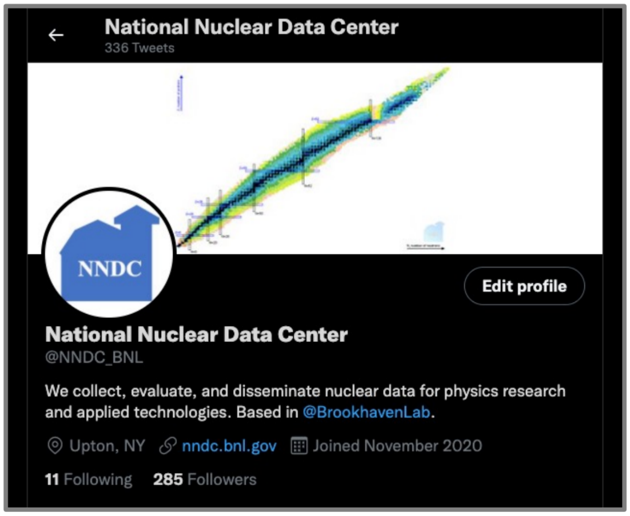
- In case of a hybrid event, remote attendees will need to pay the same registration fee.
- Smaller reg. fee will apply if the event switches to fully remote
- Remote attendees should plan to pre-record and upload talks, then participate in a scheduled Q&A session.
    - Hope to use Zoom (wider user base than Webex), requires LLNL approval
- We are considering several options for virtual poster session
    - GatherTown (https://www.gather.town), Cvent (https://www.cvent.com)

Session: Outreach

Discussion on Outreach
15:35 - 16:05
Benjamin Shu
Elizabeth McCutchan

NNDC Twitter Outreach Year 1

Yes, we have a Twitter!



Humble Beginnings:

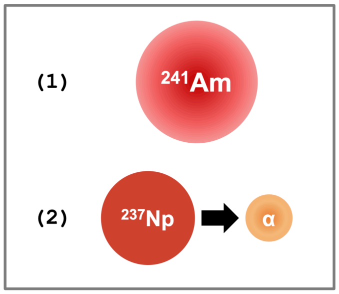
- Originally created for announcements & database updates

Video Tutorials

- #NNDCCanDo
- Short (silent) demonstrations of features on NNDC websites

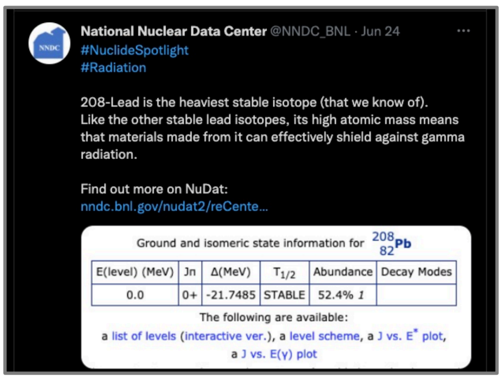
Illustrations

- #DescribeADecay
- Simple diagrams explaining types of nuclear decay



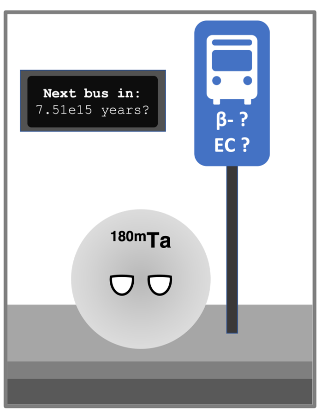
Trivia

- #NuclideSpotlight
- Describing unique traits/uses of individual nuclei…



…Comics?

- #NuclideSpotlight
- …by giving them faces and expressions?



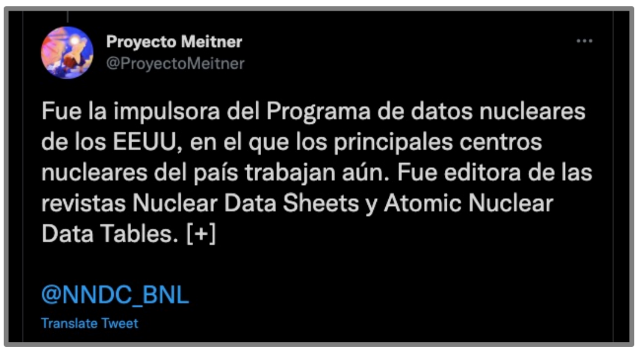
Wait, What Was the Plan, Again?

- Direction and goals for Twitter have evolved
  - Social media can reach audiences we don't normally interact with
- Opportunities for education and outreach
  - "Physics sure is interesting, isn't it? You know who could help you with that?"

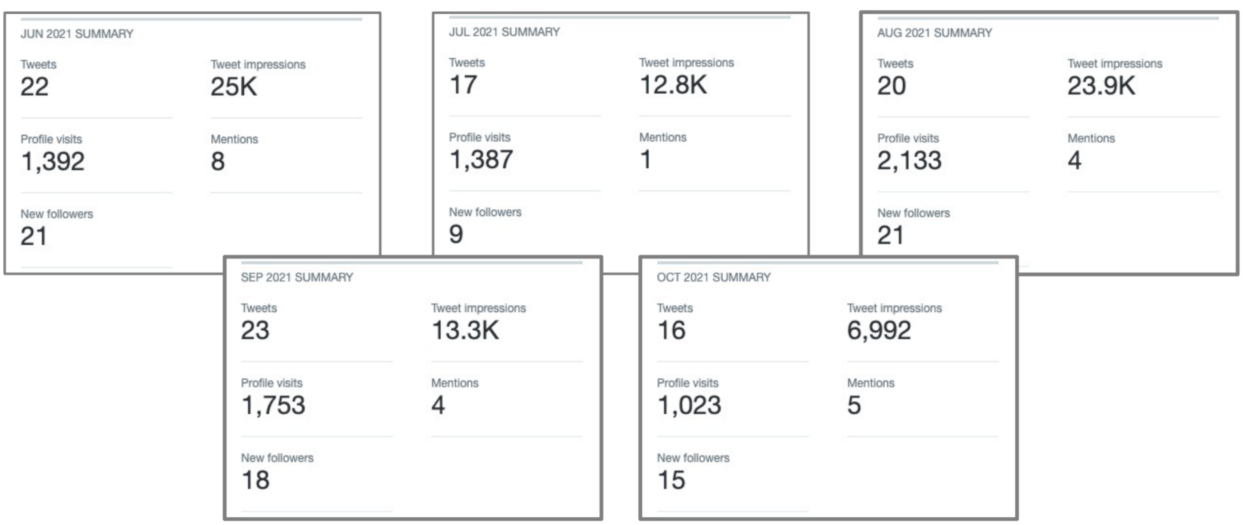
- Chances to make science more approachable and less intimidating
    - “Wait, there are good kinds of radiation? Please, tell me more!”

Oh! Hello, World!

- Our first #NuclideSpotlight was also our most popular!
- As it turns out, nuclear energy is a hot topic!
- “704 million years? I didn’t know that!”
- “Where can I find more information?”
- Twitter users mention us, ask questions and give feedback…
- …sometimes from other countries!
- Now we know about the Meitner Project
- And now their followers know about us



- Physics has a social media audience!



Why Are We Telling You This?

- We want more community involvement!
    - Promotion of other organizations/services

    - Coverage for a broad range of topics
    - Sharing of information on current research
- We want to hear from you!
    - Links, news articles, ideas for tweets, etc.
    - Tell us about yourselves, and your work!
        - Who are you, and what do you do?

What Are We Looking For?

- Short (but accurate) descriptions of services/functions
- Provide links and contact information
- Creative presentations of topics in nuclear physics
- Visuals are very good at sparking interest!
- Engagement with other Twitter users
- Answering questions, from people with or without a physics background

Dave suggested tweets about the history of benchmarks

Wednesday 17 November 2021

Session: Evaluation Committee - TSL sublibrary

Welcome to the TSL session, we have 9 talks, 1 talk will be jointly given (Andrej + Ingrid).

TNSL Implementation and Testing in FUDGE
10:00 - 10:12
Caleb Mattoon

TNSL improvements in FUDGE

LLNL infrastructure for managing and processing nuclear data

- GNDS: Generalized Nuclear Database Structure
    - New international format for storing evaluated and processed nuclear data
    - Replaces various formats including ENDF-6
- FUDGE: For Updating Data and Generating Evaluations
    - Python based code for modifying, viewing and processing nuclear data

    - Computationally intensive routines written in C and C++
    - FUDGE-5.0 now available at github.com/LLNL/fudge
- GIDI+: General Interaction Data Interface
    - Suite of C++ APIs for accessing GNDS data for use in transport codes
    - Includes API for sampling GNDS data as needed by Monte Carlo codes
    - New release coming soon to github.com/LLNL/gidiplus
- Both codes are open source and used externally

Recent FUDGE development has focused on improving low-energy neutron capabilities, especially for TNSL and URR.

- Thermal Neutron Scattering Law
    - TNSL format specification is changing significantly in GNDS-2.0
    - FUDGE processing implemented, tested various ways
        - Compare directly (processed cross sections and spectra) and indirectly (broomsticks, keff)
        - Some differences for incoherent inelastic require further exploration
    - Now have several methods for getting processed FUDGE results into transport codes
        - GNDS with GIDI+, ACE format, ENDL format with COG library generator or legacy LLNL processing
- Unresolved resonance region
    - FUDGE probability tables (especially for elastic and total) often show narrower cross section range compared to NJOY / FRENDY
    - Working with other code developers to understand that difference

The hierarchy for storing TNSL data was overhauled between GNDS-1.9 and GNDS-2.0:

- GNDS-2.0 layout integrates TNSL with all other reactions. Integrating and renormalizing TNSL double-differential cross sections produces a standard cross section and outgoing neutron distribution.

Coherent elastic: bulk scattering off crystalline materials

- Outgoing angular distribution consists of delta functions at various μi
- TODO: sample angles directly using si (T)
    - Requires some work in GIDI+

Incoherent elastic: bulk scattering off partially ordered materials

GNDS easily handles new LTHR=3 (mixed elastic) format

- Some materials require both coherent elastic and incoherent elastic (plus inelastic) to properly represent thermal scattering region.
- Handled in GNDS simply by adding another reaction node for the new elastic term
- Example files for 7LiH and 7LiD were translated to GNDS and processed with FUDGE

- Results can be translated to ENDL, ACE coming soon once we check latest format update…

Incoherent inelastic is trickier, often requires extrapolation beyond tabulated Sab grid especially at forward angles.

- A_0, M_n, $sigma_{bn}$, S_n(alpha,beta,T) are tabulated
- alpha,beta grids in many evaluations aren't sufficient for spanning all (E, E', μ) of interest
  - Short collision time (SCT) approximation is appropriate for large alpha,beta but generally not as alpha approaches 0
  - Extrapolation required for small alpha, but appears to be handled differently by processing codes
    - Especially relevant for forward scattering where E' ≈ E

Transition from tabulated S(alpha,beta) to SCT is mostly smooth at the high-a end but SCT falls off too fast at the low end.

FUDGE uses power-law extrapolation for up to 5 orders of magnitude in alpha, then switches to S = constant

FUDGE TNSL cross sections compared to NJOY Mostly agree, some differences at low incident energy…
Recent update: iteratively add points to refine cross section

Recently switched incoherent inelastic distribution storage from P(E'|E,μ) to P(μ|E, E')

- P(E'|E,μ) originally used for compatibility with legacy LLNL format ENDL, but storing a μ distribution for each incident / outgoing energy is more efficient

FUDGE / NJOY differences appear to originate with how each code handles extrapolation to small alpha

- Different approximations for forward scattering in H2O near E = E' = 10^{-11} MeV
  - Note: using THERMR with iform=1 option for easier comparison
- Better would be to improve documentation on how extrapolation should be done

Additional TNSL testing: run broomsticks, critical assemblies and full-scale reactor problems

- Processed GNDS data used with Mercury (MC transport) and Ardra (deterministic)
  - Results compared against MCNP/ENDF80SaB2
  - Modeled critical assemblies, ACRR reactor in several configurations
- Also exported to COG (via legacy ENDL format) for further testing by LLNL Criticality Safety group
  - Minor complication: ENDL requires P(μ | E) * P(E' | E, μ) while ACE requires P(E', μ | E)

MCNP and MCGIDI (Monte Carlo sampling library in GIDI+) handling interpolation differently

- To understand Mercury/MCNP broomstick differences, FUDGE was modified to process H in ZrH on the same incident energy grid as ENDF80SaB2 ACE files.
- Broomsticks then run with incident energies at grid points (0.95 and 1.05 eV) and at points between… results indicate an interpolation bug in MCGIDI

Conclusion:

- FUDGE TNSL processing capabilities are improving
    - New development focuses on reading and writing GNDS, but FUDGE also supports writing to ACE and ENDL
    - Work provides a chance to compare in-depth with other codes
- TNSL processing is mostly complete, but MCGIDI sampling has room for improvement
    - Revisit interpolation + improved strategies for sampling coherent / incoherent elastic

NJOY+NCrystal: Update of the Code and Thermal Scattering Library
10:12 - 10:24
Jose Ignacio Marquez Damian

Identified three weak areas: Moderators, Reflectors, and Structural and other materials

The main tool is the LEAPR module in NJOY.
• Bragg edges (Ehkl · σhkl), σ coh b and σ inc b , and σfree are passed from NCrystal
• S(α, β) (the inelastic component) is calculated in LEAPR.

Description of elastic options

Option iel =100, MEF
Simplified flow of NJOY+NCrystal when the mixed elastic option (MEF) is used

Option iel = 99, CEF (single atom case)
Simplified flow of NJOY+NCrystal when the curent elastic format (CEF) option is used for a monatomic scatterer.
Simplified flow of NJOY+NCrystal when the curent elastic format (CEF) option is used for a polyatomic or molecular scatterer.

Inelastic/Elastic calculation consistency

- LEAPR only handles the frequency spectrum of one component at a time, whereas NCrystal needs the Debye-Waller factor of all components to calculate the coherent elastic cross section.
- A consistency check is made using the mean squared displacement (MSD,hu 2 i) value for each phonon spectrum. In NJOY+NCrystal we calculate hu 2 i using LEAPR and NCrystal, and write to the output file

- Of 2523 test calculations for 213 evaluations, 2224 (88%) have a difference below 0.1%, and all of them below 0.9%.

Examples shown for MgH2 and MgD2, showing good agreement.

Another example given is Vanadium which is an incoherent scatterer, and Tin which is a coherent scatterer.

Nickel was shown as example of mixed scatterer

Validation: X-ray diffraction
Comparison of total scattering XS (left) and X-ray diffraction (right) between NJOY-NCrystal and ENDF/B-VIII.0 for 3C-SiC (β-SiC).

Cross-comparison with CINEL
Comparison of calculations with NJOY+NCrystal and CINEL of the coherent scattering component in MgH2. Thanks to Shuqi Xu from CEA-Cadarache.

Additional libraries

- Available online: https://github.com/highness-eu/NJOY-NCrystal-Library/tree/v1.3
- Version 1.3 includes adaptive alpha and beta grid, improved approximation for current ENDF format, and corrections after benchmarking with CINEL.

Conclusions

- NJOY+NCrystal is a user friendly, open source tool for the generation of TSL libraries for ordered materials.
- This tool was used to generate 200+ evaluations for 100+ new and updated materials, validated against total cross sections, specific heat capacity (Cp) measurements, and X-ray diffraction.
- From the first release back in May there were significant improvements in the code and the library.
- This improvement was benefited from cross comparison with different codes and libraries.

Nuclear Graphite TSL Evaluation and Cross Section
10:24 - 10:36
Iyad Al-Qasir

Nuclear Graphite Manufacturing Process

- Calcination process between 900 and 1300 °C to remove volatile materials and to reduce the amount of shrinkage

- The calcined coke is then crushed, milled, and blended with a graphitizable pitch to facilitate the forming of the filler-binder mixture.
- The green article baked between 800 and 1000 °C to convert the binder from a thermoplastic material to an infusible solid as well as to release H and vent the volatiles
- The release of hydrogen gas during the baking process creates pores, which can vary in size and type
- During graphitization process (2500-3000 C), as the temperature reaches 1500 °C most of the hydrogen will be evolved , between 1500 and 2500 °C the graphite crystals will start to be formed and above 2500 °C diffusion and annealing out of crystallite imperfections will improve the graphitic crystal structure of both the coke and binder

Nuclear Graphite has a complicated structure

Graphite Samples:

- Focus on two types of graphite
  - G347A
  - PGA

It shown:

- Workflow illustrating the scheme of work
- Examples of measured and calculated scattering functions S(Q,E)
- Measured and calculated PDOSs
- Excellent agreement between the different types graphite and good agreement with the calculated
- Measured & Calculated Double Differential Scattering Cross Sections
- Cross Sections
  - Good agreement of the calculated cross sections at all temperatures

Conclusion

- The inelastic neutron scattering technique was successfully used to measure the scattering functions, double differential scattering cross-sections as well as the full phonon density of states of the G347A and PGA nuclear graphite at room temperature.
- Excellent agreement found between the measured scattering functions of nuclear graphite (G347A and PGA) and calculated scattering functions of theoretical graphite
- Excellent agreement between the calculated graphite cross section including the coherent one phonon and the measured data of HOPG and AGOT graphite.
- The high cross section of nuclear graphite cannot be attributed to neutron-phonon interaction, it is due to the small angel neutron scattering

Exposed to different radiation temperatures

Comment from Ayman: The material is porous and the modeling should account for that porosity. If they show small angle scattering that means the material is porous. If we know the material is porous, do you capture this porosity?

Code Verification Project for Generating ACE Libraries
10:36 - 10:48
Dr Andrej Trkov
Zirconium Hydride TSL Evaluation
11:00 - 11:12
Ingrid Švajger

Thermal Scattering Law Data for ZrH

IAEA Code Verification Project for processing evaluated nuclear data into ACE format

- Stage-1: Processing cross sections, differential and double-differential data (9 codes participated, done)
- Stage-2: Preparation of probability tables / multi-band parameters (done)
- Stage-3: Processing of thermal scattering law data (7 codes participated https://www-nds.iaea.org/index-meeting-crp/TM-NDP-2021/)
    - Progress considering that for so long only NJOY was able to produce ACE files
- Stage-3: Thermal scattering law
    - Preference was given to TSL processing for Stage-3 so that thermal systems could be analyzed
    - Test case: H in ZrH from the ENDF/B-VIII.0 library
    - Selected benchmarks from the ICSBEP Handbook containing ZrH (15 cases)
    - Note that two formats exist for TSL-ACE designated by IFENG=1 or IFENG=2 flag
    - The latter (continuous energy) is favoured.

Presented

- list of benchmarks involving H in ZrH
- list of participating codes
- Benchmark results with ACE-TSL formatting option IFENG=1 and 2

New TSL evaluations for ZrH

- Work is in progress by Ingrid Švajger from JSI (in collaboration with NCSU) on ZrH TSL data from first principles
    - Preliminary file for H in ZrH_2 is available
- Work on ZrH was published by Tiejun Zu et al. from Xi'an Jiaotong University (XJTU) (ANE 161 (2021) 108489)
    - Files for H in ZrH_2 and H in $ZrH_{1.5}$ were provided for testing

    - Input models for HCM003 were provided (ICSBEP Handbook only gives Case-1)

Atomic Structure – ZrH_2
- Tetragonal crystalline structure
- Zr at (0, 0, 0)
- H at (0, ½, ¼)

Phonon density of states – ZrH_2
- Weaver J H, Peterman D J, Peterson D T and Franciosi A 1981 *Phys. Rev.* B *23* 1692.
- Evans, A., Timms, D., Mayers, J., Bennington, S., 1996. Neutron-scattering study of the impulse approximation in ZrH2. Phys. Rev. B - Condens. Matter Mater. Phys. 53, 3023–3031.

Observations:
- IAEA Project on data processing for ACE libraries provides guidelines for accurate processing and particularly for the use of the continuous energy (IFENG=2) format option
- Local processing of H in ZrH with NJOY agrees reasonably with the results using the official SAB2 library from LANL
- **New** evaluations for the TSL of ZrH are available and are being tested on a selection of ICSBEP benchmarks
- HCM003 benchmarks (Narcis-M) have H/Zr ratio of 1.92 – calculations with TSL for H in ZrH2 from JSI and XJTU agree with each other and with the measured values
- TSL for H in ZrH1.5 from XJTU gives results very close to the original LANL SAB2 data from the ENDF/B-VIII.0 library
- ICT013 benchmarks (NRAD TRIGA containing Er) remain strongly discrepant with all TSL data.

Jonathan Wormwald mentioned that there is a ZrH2 in VIII.0.
Zerkle: HCM003 is the best benchmark for epsilon phase

Thermal Neutron Scattering Evaluation for Polyethylene from RPI/ORNL/ESS
10:48 - 11:00
Kemal Ramic

Most of this was presented in mini-CSEW but there are new things to show

Introduction
- In the absence of phono spectrum (VDOS) based scattering kernels, thermal neutron scattering can be sampled using
    - Free gas model

- Debye model:
  - Idealized DOS (Debye Model) is constructed and fed into same infrastructure as any other DOS.
  - Lacks details of course, but gives consistent kinematics and handles multi-phonon physics rather well.
- But with the availability of the phonon spectrum
- But only phonon based scattering kernels correctly calculate microscopic quantities
- The scattering kernel with best predictive capabilities will have an accurate calculation of integral and microscopic quantities as well.

Inelastic Physics

- All the modeling techniques calculate only fundamental vibrational mode (n=1) phonon spectrum!!!
- https://doi.org/10.1016/S1369-7021(05)71336-5 - "Neutron scattering and hydrogenous materials"

Revisiting Polyethylene

- Comparison with experimental S(Q,ω) from VISION instrument
- Fundamental vibrational mode vs multiple phonon contributions
- Experiments measure phonon spectrum with multiple phonon contributions included (n»1)!!!
- Can ENDF phonon spectrum result in the same S(Q,ω) as measured at VISION?
- New method by Dr. Chapman extracts S(α, β) from an ENDF file at a trajectory in S(Q, ω) phase space that corresponds to one neutrons would travel at VISION instrument at SNS at ORNL, converts it to S(Q, ω), and applies instrumental resolution.
- Direct geometry instrument S(Q,ω) phase space (ARCS or SEQUOIA)
- Indirect geometry instrument S(Q,ω) phase space (VISION)
- New RPI Polyethylene total cross section data measured typical High Density Polyethyelene (HDPE). • We can separate the VDOS into distinct regions and optimize until agreement with the cross-section matched as best as possible.
- We used NCrystal and Dakota to minimize χ 2 between the RPI new data and the evaluation. The weights for each region where changed by Dakota, total cross section is calculated by NCrystal at exactly same energy grid as the experimental cross section data, and χ 2 was calculated. The process was repeated until optimal minimal difference in χ 2 was achieved.

Showed plots of:

- HDPE total cross section (1e-7 to 10 eV)
- HDPE total cross section (1e-7 to 1e-5 eV)
  - Y. N. Pokotilovski et al., "A differential time-of-flight spectrometer of very slow neutrons", Instruments and Experimental Techniques, vol. 54, pp. 16–22, 2011
- HDPE total cross section (1e-3 to 10 eV)
- HDPE total cross section (1e-3 to 5e-2 eV)

- HDPE total cross section (2e-2 to 2e-1 eV)
- RPI experiment HDPE C/E-1

Microscopic level: RPI/ESS/ORNL PE scattering kernel has better predictive capabilities on both microscopical and integral level.

Polyethylene as a perfect crystal:

- Polyethylene is after all crystalline material, so coherent elastic effects should be taken into account. HDPE is up 80% crystaline material.
- Because Polyethylene isn't made of perfect crystals, extinction could be a possible explanation.
- D. D. DiJulio et al., "Impact of crystallite size on the performance of a beryllium reflector", Journal of Neutron Research, vol. 22, no. 2-3, pp. 275-279, 2020

Conclusions

- The importance of microscopic quantities has been demonstrated for the accurate predictability of thermalization of neutrons
- RPI Polyethylene library has been revisited (merged into Phase 1, with C in CH2 for completeness) and shown to be in the best agreement with available relevant experimental data
- A new path for validation of tsl-ENDF files has been proposed starting from phonon measurements to total cross section measurements. Tools such as VISION, ARCS and SEQUOIA spectrometers at ORNL, should be part of validation and evaluation of thermal scattering libraries

Evaluation of the Thermal Neutron Scattering Cross Sections of CaH2

11:12 - 11:24

Benjamin Laramee

Introduction

- Metal hydrides have long been considered and used as moderator materials
    - High hydrogen content
    - Good thermal stability
    - Relatively low neutron absorption
- ZrH2 TRIGA Reactors
- Kimura &Wada (2016-2019)
    - CaH2 -moderated microreactor (<10 MW)

Existing CaH2 Data

- Very little experimental data overall, including :

    - Cross Sections
    - Phonon DOS (vDOS)
    - Crystal, Material Properties
- Existing Cross Section Data :
    - No ENDF Evaluation to date
    - JEFF3.1 (O. Serot, 2005) -> JEFF3.3
        - Contains significant physical approximations
- W. M MUELLER et al., Metal Hydrides. New York: Academic Press, Inc. (1968).

JEFF3.3 Data

- O.SEROT, “New results on CaH2 thermal neutron scattering cross sections,” AIP Conference Proceedings, 769, 1, 1446 (2005).

Evaluation Process

- Approximations
    - Incoherent approximation: Sd (alpha, beta) =0
    - Gaussian
        - Harmonic

CaH2 Crystal Structure

- Orthorhombic (Pnma)
- 3 non-equivalent atom sites: Ca, H_1 , H_2
- VASP DFT Model:
    - GGA-PBE, 675ev PW Cutoff, 9x9x9 Monkhorst-Pack k-point mesh
- H. Wu et al., “Structure and vibrational spectra of calcium hydride and deuteride,” Journal of Alloys and Compounds, 436, 1-2, 51(2007)

Phonon DOS

- PHONON : 3x3x3 Supercell (324 atoms)
- P. MORRIS et al., “Inelastic neutron scattering study of the vibration frequencies of hydrogen in calcium dihydride,” Journal of Alloys and Compounds, 363, 1-2, 88 (2004).

FLASSH: Full Analysis Scattering System Hub

- Motivation - provide cross section data to support advanced reactor modeling and criticality safety
    - High Fidelity – TSL calculations with modern coding techniques using advanced physics
    - Advanced Physics – distinct (1- phonon) contributions and noncubic formulations
    - Graphical User Interface – makes complex physics accessible to all users
    - Convenient Output Formatting – user output files, ACE files, plotted data, etc.
- Advanced TSL capabilities :
    - automatic α, β gridding

    - read existing TSL to calculate cross sections
    - Loosening of the incoherent approximation: $S = Ss + Sd$ 1
    - Doppler broadening capability
- Cross Sections :
    - Coherent elastic for any material
    - Noncubic formulation
    - Mixed elastic
- Making the evaluator's job easier:
    - GUI
        - Comprehensive error checking
    - Built-in ENDF/B-VIII.0 materials
    - Convenient formatting options
        - ENDF-6 File 7 (w/ MF=1,MT=451)
        - ACE (w/ mixed elastic)
        - NJOY-LEAPR input tape
    - Plotting
        - α, S α, β for select β
        - β, S α, β for select α
        - Cross Sections
            - Temperature comparisons for all data
            - All contributions and total cross section
    - FUDGE/GNDS Compatibility
        - C++ GUI & Python

CaH2 TSL for ENDF Consideration

- The following 3 evaluations have been submitted to the NNDC for consideration for ENDF/B-VIII.1:
    - Ca in CaH2 (MAT=59)
        - MT = 4 (Coherent)
        - MT = 2
    - H1 in CaH2 (MAT=8)
        - MT = 4 (Incoherent)
        - MT = 2
    - H2 in CaH2 (MAT=9)
        - MT = 4 (Incoherent)
        - MT = 2

Summary

- CaH2 evaluation was performed using the FLASSH code
    - Evaluated the coherent elastic component of Ca in CaH2
    - Evaluated the cross sections for the nonequivalent H1 & H2 atom sites, as opposed to an averaged H

- Accounted for the negative coherent scattering length of H

Evaluation of TSL of the delta-phase yttrium hydride (YH2 to YH1.31)
11:24 - 11:36
Vedant Mehta

Y-H phase diagram: Motivation from mircoreactors

YH_2 phonon density of states benchmark calculations

- Excellent agreement with Zerkle et al. phonons
- Large mass difference causes large frequency gap
- Hydrogen predominantly vibrating in optical range
- Yttrium predominantly vibrating in acoustic range
- References:
    - M. Zerkle and J. Holmes, EPJ Web of Conferences, vol. 146 (2017)
    - D. A. Brown et al., NDS 148 (2018) 1-142

Benchmark with ENDF/B-VIII.0
Process: SQS-ATAT -> VASP (DFT) -> NJOY16; incoherent approximation

Point defects in YH_2 – first step to YH_{2-x}

- Firstly, the positive energy to form a Frenkel defect in YH2 confirms H is stable at the tetrahedral site and unstable at the octahedral site – YH2 is fluorite
- Small deviations from YH_2 to YH_{2-x} are studied through three possible mechanisms under U-rich conditions by which YH_2 can become YH_{2-x}: hydrogen vacancy, antisite, and Yttrium interstitial
- The hydrogen vacancy at the tetrahedral site is dominant in YH_{2-x} – this will be used as basis for bigger deviations H/Y
- The small positive formation energy indicates Y metal + YH_2 at low temperatures in line with the phase diagram

Thermal Scattering Laws

- The phonon spectrum for the defective supercells for $YH_{1.31-1.91}$ has been used to evaluate neutron thermal scattering laws (TSLs) for use in MCNP
    - TSLs provide the interaction probability of an incident neutron with target nucleus at thermal energies
    - TSLs differ from free gas XS as they rely on the molecular structure of the compound
- For significant sub-stoichiometries, the molecular structure, and thus TSLs differ
- Due to predominance of hydrogen, incoherent approximation was used.

Phonons at sub-stoichiometry

- Special Quasi-random Structures provided 5crystal structures for individual stoichiometry
- Energy minimization provided the lowest energy structure
- Phonons calculated for the lowest energy structure
- Phonon calculations applied to a wide range of compositions of YH_{2-x}
- Removal of H causes phonon splitting in the phonon dispersion curves

Crystal structure and phonons benchmarked at several stages

- Benchmark against literature data and neutron diffraction data
- Cp and thermal lattice strain comparison with experiments
- Atomic displacement parameter comparison

Thermal Scattering Laws: New evaluations

- Novel TSLs for significant sub-stoichiometries were developed and are planned to be released in the next ENDF evaluation
- Phonon DOS were used to generate the TSLs between stoichiometries $YH_{1.31}$ to YH_2
- Deviations up to ~60% at most probable energies observed in the new TSLs

New evaluations published in NSE

- V. K. Mehta et al., NSE 195.6 (2021): 563-577

Future work: Inclusion of coherence for Y in YH2-x using NJOY-Ncrystal (arXiv:2108.11737 (2021))

Zirconium Carbide TSL Development

11:36 - 11:48

Jonathan Wormald

Overview

- Zirconium Carbide (ZrC) is a refractory material currently investigated for high temperature reactor applications
    - Fission product barrier in advanced TRISO
    - Corrosion barrier in space nuclear thermal propulsion (SNTP)
- ZrC studied as base of (U,Zr)C solid solution and UC2 composite fuels for NERVA-type cores during Rover program
    - Testing of material performed at Nuclear Furnace 1 (NF-1) located at Los Alamos
- Thermal Scattering Law (TSL) evaluations generated with FLASSH as new contribution to ENDF/B-VIII.1

- Standard incoherent approximation
- New mixed elastic scattering format
- Disordered alloy theory introduced to coherent elastic scattering to capture natural isotopic abundances
- Work submitted to PHYSOR 2022

Zirconium Carbide Phonon Model Validation

- Crystal structure lattice parameter in agreement with experiment.
  - 0.471 nm vs. 0.470 nm
- Phonon dispersions relations in good agreement with experiment
  - Differential validation of phonon spectra
- Debye-Waller coefficient in reasonable agreement with experiment from 0 K – 1600 K
  - Integral validation of phonon spectrum
  - W is a measure of mean square displacement used directly in TSL
- C(ZrC) spectra localized around higher energy modes separated from lower energy modes
  - Similar behavior in metal-hydrides introduce regular structure $S(\alpha, \beta)$ (quantum oscillations) that strongly influence thermalization

Thermal Neutron Scattering Formalism

- TSL contains distinct (interference) and self (non-interference) components
  - Momentum transfer (α) and energy transfer (β) represented with unitless parameters
- Phonon expansion used in incoherent approximation for inelastic scattering ($p > 0$)
- C(ZrC) and Zr(ZrC) both include: coherent elastic, incoherent elastic, and inelastic
  - 91Zr and 13C have small incoherent nuclear potential
  - Disordered alloy theory invoked to treat coherent elastic

ZrC TSL Evaluation Parameters

- C and Zr potential scattering cross sections extracted from ENDF/B-VIII.0 nuclide evaluations at incident neutron energy of 0.0253 eV
  - Incoherent cross section from V. F. Sears, Neutron News, 29, (1992) 26-37
  - Isotopic average cross section for incoherent elastic and inelastic scattering
  - Isotopic average scattering length for coherent elastic scattering
- C(ZrC) and Zr(ZrC) evaluated at 13 temperature:
  - 77 K, 293.6 K, 400 K, 500 K, 600 K, 700 K, 800 K, 1000 K, 1200 K, 1400 K, 1600 K, 1800 K, 2000 K
- Phonon expansion order of 300 used for convergence of $S\ \alpha, \beta$
  - Eliminate the need for short collision-time-approximation in FLASSH
- (α,β) grid valid to 5 eV incident neutron energy
  - Default automatic grid in FLASSH
  - α-grid of 200 points 0.415322/A , 790.5139/A
  - β-grid of 283 points 0,197.63

ZrC TSL Evaluation

- Zr(ZrC) TSLs characteristic of heavy elements in crystalline compounds
    - Structure up to 1-phonon energy transfer and relatively featureless beyond
    - Approximating free-gas (FG) for high momentum transfer
- C(ZrC) has strong quantum oscillator effect to multiple phonon orders
    - Oscillations in TSL correspond to phonon order
    - Energy transfer involves quantized exchange of higher energy phonons with substantial downscattering and upscattering
        - Differs from H(ZrHx) where upscattering is unlikely at room temperature
    - Shallow oscillations persist as FG behavior present for large momentum and energy

C(ZrC) Secondary Neutron Distributions

- C(ZrC) is compared to reactor-grade graphite (RxGr)
    - RxGr represents conventional TSL for chemical binding of C
- Epithermal range: ZrC down-scattering is quantized and greater than RxGr
    - Behaviors more similar at higher temperature but some quantization remains
- Neutrons in the phonon energy range have unusually probable high energy losses
    - Near complete energy loss
        - Atypical of non-hydrogenous solids
    - Improbable for FG or typical carbon compounds
- Thermal range: Quantized energy loss is forbidden in thermal energy range and below
    - Up-scattering is dominant
        - Spectral hardening is expected
    - Increase probability of quantized upscattering with temperature
        - Consistent with metal hydrides

Conclusions

- New TSL evaluations for ZrC have been generated for contribution to ENDF/B-VIII.1
    - Support criticality safety analyses for high temperature reactor systems
- New evaluations extend physics of elastic scattering used in ENDF evaluations
    - Use of mixed elastic scattering
    - Introduction of disordered alloy theory to improve coherent elastic treatment
- C(ZrC) exhibits quantum oscillator behavior that is atypical of nonhydrogenous compounds
    - May be important for evaluation of systems with significant ZrC content
        - TRISO coatings
        - SNTP applications
    - Initial critical mass calculations demonstrate a C(ZrC) impact compared to FG
    - Further effects testing is in progress

Uranium Carbide and Uranium-Metal TSL Evaluations and Cross Sections
11:48 - 12:00
Jonathan Crozier

Motivation

- TSL describes scattering system: impacts neutron thermalization and may inform resonance broadening
    - TSL impacts thermal cross sections, thermal neutron spectrum, criticality safety, Doppler broadening
- Generate ab initio thermal scattering cross sections for advanced reactor fuel materials: Uranium Carbide and Uranium Metal
    - UC and U-Metal have high thermal conductivities and fissile isotope densities
    - UC considered for thermal nuclear propulsion, HTGR TRISO fuel particles, fast breeder fuel

Uranium Carbide AILD

- VASP DFT framework
    - GGA-PBEsol Pseudopotential
    - 1.9 eV Effective Hubbard Term
    - Magnetic structure capture with Spin-orbit-coupling
        - AFM-I polarizations in x, y, z -> PM
    - 2x2x2 Supercell, 64 atoms
    - .02 angstrom displacements in +/- x-direction for non-equivalent sites

Uranium Carbide TSL at 296 K

- Uranium in UC
- Carbon in UC
- Evaluated for 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000K

File submitted to NNDC

Uranium Metal AIMD

- Ab inition Molecular Dynamics
    - Ab initio required to capture accurate electronic structure
    - MD required to capture temperature dependence
- VASP Molecular Dynamics Inputs
    - GGA-PBE pseudopotential
    - No Hubbard corrections or spin-orbit coupling
    - 5x2x3 Supercell, 120 Atoms
    - 0.05fs timestep
    - 296K
    - 3ps – equilibration

- 10ps – VACF calculation

Uranium Metal TSL at 296K

- Evaluated for 296, 400, 500, 600, 700, 800, and 900K
- Alpha-phase stable up to ~668 degrees Celsius
- Room temperature traditionally used in cross section measurements

Uranium file also submitted to NNDC

Summary

- New Uranium Carbide and Uranium Metal evaluations using the FLASSH platform
  - Ab initio LD/MD models – converged electronic, magnetic and dynamical properties demonstrate good agreement with experimental data
  - Thermal scattering cross sections – generate inelastic and elastic thermal neutron scattering libraries in FLASSH
  - New TSL evaluations – production of ENDF file 7 data for Uranium Carbide and Uranium Metal submitted to NNDC for ENDF/B-VIII.1 release
- Presented list or TSL evaluations 2020-2021
  - Some of these evaluations include new Physics

Session: Evaluation Committee - Fission Product Yields

Nuclear Data Activities on Fission Yields at LBNL
13:00 - 13:20
Eric Matthews

Fission Yield Measurements at the Fast Loading User Facility for Fission Yields (FLUFFY)
FLUFFY

- The Fast Loading User Facility for Fission Yields (FLUFFY) was developed at LBNL to rapidly shuttle actinide samples between a neutron source and counting array.
- Transport times of
- Flux: 7.2 x 10^8 n/cm2/s
- This high flux along with the rapid transport time allows for the observation of 80+% of the yield in peak mass chains.

July 2020 Experiment

- On July 21-26, 2020, 238U and 235U samples were irradiated at the Fast Loading User Facility for Fission Yields (FLUFFY) at LBNL’s 88-inch cyclotron.
  - 24 hours of 1 s-25 s 238U data (455.3 mg)

- 24 hours of 5 s-125 s 238U data (455.3 mg)
- ~16 hours of 1 s-25 s 235U data (~20 mg)
- Neutron energy spectrum data for 14 MeV deuteron breakup on graphite
- 8 hour foil pack irradiation
- Single nTOF irradiation

The Experimental Data

- The experimental data produced by FLUFFY is □ emissions as a function of time since irradiation start, time since capsule arrival at counting station, and as a function of the emitting product isotope

The FIER Model

- The Fission Induced Electromagnetic Response (FIER) code offers a model that produces analogous FPY gamma emission data.
- Chi-squared minimization between FIER and experimental data is used to determine fission yields and correct decay data

Mass Chain Analysis: Example given for A = 86

High 1564.64 keV -energy gammas have lower backgrounds!

Results

- An example of results from the A = 86 mass chain
- Number of emission plots shown for A = 86:
    - Emissions of 1564.0 keV □'s from 86Br as a function of time since capsule arrival fit with FIER. 238U(n,f) data. FPY = 0.18% Not previously measured!
    - Emissions of 2660.0 keV □'s from 86Se as a function of time since capsule arrival fit with FIER. 238U(n,f) data. FPY = 1.05% □) = 24.9% (↑11%)
- Gamma emission rates from the daughter FP simultaneously constrain the FPY and □# of the parent.

Fission Yield Correlation/Covariance Matrices

Motivation:

- Neither the ENDF/B-VIII.0 or JEFF-3.1 fission yield evaluations include information on covariances between fission yields. [1,2]
- Covariances between fission yields affect several important applications:
    - Forensics and safeguards calculations
    - Reactor antineutrino rates
    - Reactor inventory, decay heat, and poisoning

[1] – Evaluation and Compilation of Fission Product Yields – T.R. England and B.F. Rider (1994)
[2] – R. W. Mills, Fission product yield evaluation, Ph.D. thesis, University of Birmingham (1995)

Previous Work:

- Pigni et al. – 2013

    - Variance estimation with Wahl systematics
- Schmidt – 2013
    - Parameter perturbation in the GEF code
- Leray et al. – 2017
    - Parameter perturbation in the GEF code
- Kawano and Chadwick – 2013
    - Bayesian method for 239Pu FPY
- Work by Pigni, Schmidt, and Leray relies on an underlying model of fission and parameter uncertainties.
- Results of these work are not readily accessible due in part to ENDF format limitations.

Motivation:
- The goal of this work is to generate a set of covariance matrices for the fissioning systems of a given fission yield evaluation with as little fission model bias/uncertainty as possible.
- This method seeks to use simple conservation rules in order to constrain a sample space for Monte-Carlo estimation.
- The resulting covariance matrix will predominantly reflect the evaluated uncertainties in the independent fission yields.
- Public availability of the covariance matrices is a high priority.

Conserved Relationships:
- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1].

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

Conserved Relationships:
- In order to obtain correlation, conserved quantities can be enforced upon a set of resampled fission yields [1]:
    - Total Yield
    - Total Charge
    - Total Mass
    - Charge Parity
    - Mass Symmetry

[1] - Generation of Fission Yield Covariances to Correct Discrepancies in the JEFF Fission Yield Library – L. Fiorito et al. (2015) - https://www.oecd-nea.org/science/wpec/sg37/Meetings/2015_May/SG37_8_LF.pdf

FY Covariance Matrix Generation

The way in which a set of fission yields are resampled can be structured to conserve these relationships:

1) Randomly selected the “light” or “heavy” side of the fission product spectrum to resample.
2) Randomly select (weighted by uncertainty) a product in each □ chain, resample its yield about its evaluated uncertainty.
3) Scale all other yields in that □ chain by the same percent change.
4) Normalize the resampled yields such that they sum to 1.
5) Generate the fission yields on the complementary side of the fission product spectrum using the neutron multiplicity of the compound system.
6) Repeat steps 1-5) N times. Select N such that statistical noise is minimized.
7) Calculate the resulting correlation matrix from the N trials.

Step 3 is allowed if the Z distribution for a given A is Gaussian, which empirical data and the ENDF/B-VII.0 evaluation supports [1].

[1] – Evaluation and Compilation of Fission Product Yields – T.R. England and B.F. Rider (1994)

By Step 5 we’ve ensured all of the conservation rules are met.

Example: 135Te

- Presented is the covariance between independent yields as function of Z and A and that of 135Te.
- The evaluated yield for 135Te is 2.47 ± 0.57%
- Features:
  - 135Te is positively correlated with itself.
  - Products along the A chain have positive correlation.
    - This positive correlation is reflected along a complementary A = 99 chain.
  - Products along A chains that do not have complementary Z have negative correlation.

Conclusions:

- A model-agnostic method for independent fission yield covariance matrix generation is being developed.
- This method has been successfully applied to all compound systems in the ENDF/B-VIII.0 and JEFF-3.1 evaluations.
- The results demonstrate expected behavior and trends.
- Final results serve as an interim solution for independent fission yield covariance matrices until a new evaluation is completed.
  - The results are publicly available at nucleardata.berkeley.edu/FYCOM
  - Publication accepted to Atomic Data and Nuclear Data Tables on April 20, 2021.

Energy Dependent Fission Product Yields from Neutron- and Photon-Induced Fission

13:20 - 13:40
Anton Tonchev

Outline:

- Motivation:
    - Energy-dependent FPYs with broad range of half-lives form broad range of monoenergetic neutron beams
- Recent Experimental Studies and results:
    - Energy dependencies of cumulative fission-product yields from neutron induced fission on 239Pu, 235U, and 238U
    - Energy and time dependent short-lived fission product yields
    - Photofission product yields from 240Pu in comparison with neutron induced fission from 239Pu
- Summary

Review of the fission process

Long-Lived FPY Measurements at UNL using Monoenergetic neutron Beams

Cumulative FPYs at 11 incident neutron energies on 235,238U and 239 Pu

- Peculiar energy dependency
- There is a positive slope of the 147Nd FPY from 0.5 to ~4.0 MeV
- At higher energies the FPY for 147Nd turns over and decreases

Cumulative fission product yields from 235U(n,f), 238U(n,f), and 239Pu(n,f)
This peculiar energy dependency holds, examples given for 95Zr, 97Zr, 99Mo, 140Ba, 143Ce, 147Nd.
There is a gap in the mid-energy region that they want to cover in this fiscal year.

Short-lived FPYs from neutron induced fission of 235,238U and 239Pu at En = 4.6 MeV; fission product yield data with half-lives from minutes to hours

Very short-lived FPY measurements at TUNL using RABITTS
Tunnel length 10 m
FPY data for FPs with half-lives of sub second to a few minutes
Developed analytical methods to process complex gamma-ray spectra

Extending our cumulative FPY data toward independent yields

- Determined over 60 short-lived fission products with half-lives from seconds to minutes on 235,238U and 239Pu at 5 incident energies (0.5, 2.0, 4.6, 9.0,14.8 MeV)
- Measured isomeric fission-yield ratios for a handful of FPs to support theory assessment on fission fragments angular momentum

- Collaborate with NNDC and nuclear data evaluation groups to identify the most important FPs contributing to the reactor anti-neutrino anomaly and the so called "bump"

First Measurements of the Very Short-lived FPYs for fission with a monoenergetic photon beam

- More than 30 cumulative FPYs for 235U, 238U, and 239Pu for half-lives from 1-600s
- Connecting independent isotope production to cumulative yields

Try to produce the same compound nucleus and match the energy of the compound nucleus

Unique capabilities: monoenergetic neutron and gamma-ray beams at TUNL

240Pu(g,f) results at E_{gamma} = 11.2 MeV – 38 Unique FPYs

FPYs from 240Pu(g,f) at E_{gamma} = 11.2 MeV in comparison to 239Pu(n,f) at E_n = 0.5 – 14.8 MeV

- Compare 38 unique FPYs from both data sets
- 239Pu(n,f) at En = 4.6 MeV is the best fit
- 240Pu(g,f) FPY measurements test Bohr hypothesis to new level of precision in fission reactions by comparing fission yields
    - Validate ^{A}X(g,f) as surrogate for $^{A-1}$X(n,f)
- Future 240Pu(g,f) FPY measurements at additional Egamma fould further test if energy evolution of yields is consistent with Bohr hypothesis (8 MeV and 15.6 MeV data collected)

Summary: Fission product yield real estate map

Update on short-lived and cumulative fission product yields from the NPML Collaboration
13:40 - 14:00
Jason Harke
Update on short-lived and cumulative fission product yields from the NPML Collaboration
J.T. Harke, B. Bandong LLNL T.A. Bredeweg LANL
B. Pierson, J.Friese PNNL

Multi-Lab multi-disciplinary collaboration: LLNL, LANL, PNNL, Oregon State

Motivation:
There have been few short-lived fission product yield studies since the publication of the England and Rider report in 1993 (28 years). The yields in the England and Rider report are a collection of results from experiments occurring from the 1950s through to the early 1990s. Integral cross-section measurements in unperturbed fast fission neutron fields are rare but crucial data for a range of applied fields (criticality safety, reactor operations, etc...)

Approach:
Project is conducting the first set of self consistent irradiations of major actinides in nearly 30 years using:

- Long irradiations with fission chambers for an absolute fission basis estimate of yields
- Long irradiations of high purity mixed foil sets for cross-section measurements
- Prompt (< 60 µs) fission neutron bursts for relative fission yield measurements

High quality nuclear data essential to data evaluation and modeling;

- Improve nuclear data libraries
- Provide valuable nuclear data references for the nuclear science community

Neutron Sources
Operations conducted at the NCERC include both subcritical and critical experiments with the ability to measure a wide variety of nuclear properties.
Flattop (NCERC)

- Fast/fission Spectrum
- Horizontal (“traverse”) glory hole • 1013 fissions/g on samples

Godiva IV (NCERC)

- Fast/fission neutron spectrum
- Super-Prompt Critical Operations • Vertical glory hole for samples
- 1-4 × 1016 Total Fissions / burst

D-T Generator (PNNL)

- Thermo D711 neutron generator
- Low scatter facility at PNNL
- Max neutron flux of 1×10! n/cm2/s
- New D-T source at LLNL Jan-2022

Timescales of isotopes we can investigate
Fission product isotopes cover a wide range of time scales from microsecond to day++ half-lives.
We can currently make measurements:
At the 10s of minutes time scales by whole gamma counting
Hours/days by performing radiochemistry and
beta/gamma counting

Short-Lived Fission Product Yields (SLFPY)
Np237 Data Time Dependent Spectra Example

- Currently, we can retrieve the sample from Godiva ~30-40 minutes after the burst mode operation. Then begin measuring gamma-ray spectra at about 1 hour.
- Fit a peak in each in time bin and plot the intensity versus time (decay curve) — Use half-life and γ-ray energy to identify isotope
- Use decay curve to extract the activity of the isotope immediately after irradiation

Technical Approach: identifying gamma rays

Time dependent gamma ray spectra from 45 minutes to 7 days post-irradiation

List mode data taken with high resolution HPGe detectors to perform the gamma-ray spectroscopy is essential to unfolding the very complex spectra obtained from fission products.

237Np yields for 93Y as example

Results for 237Np FPYs

- Fission Product yields for 45 unique isotopes/isomers have been measured
  - Using 191 different γ-rays
  - Isomer Yields
- Half-lives ranging from 10s of minutes to a few days.
- Use multiple γ-rays from each decay if possible
  - Reduces sensitivity to systematic uncertainties introduced by potentially imprecise nuclear data
- Using multiple γ-rays can highlight areas where current evaluated branching ratios may be incorrect
- Example: 129Sb
  - Using the 761.3 keV γ-ray to measure FPY would produce a different result
  - The other 3 observed γ-rays produce a consistent value for FPY
- Indicates that there could be an issue with the branching ratio for the 761.3 keV γ-ray
  - In this case it appears that the ENSDF/B VIII.0 FPY value was measured using the 761.3 resulting in an inaccurate FPY

Integral measurement of 237Np(n,g)238Np cross section

g-rays form decay of 238Np **were observed in the time dependent spectrum**

activity of 238Np used to determine amount produced during irradiation

NCERC Flattop assembly irradiation and modeling to evaluate the 9Be(n,g**)10Be cross section at fission energies**

Courtesy of Jack Goodell, Jennifer Church and Bryan Bandong

- High-fidelity model of the Flattop assembly and experimental configuration simulated using MCNP6.2
- 9Be(n,g)10Be integral cross section determined by total neutron fluence and the 10Be/9Be ratio
- Neutron fluence estimates determined by 197Au(n,g)198Au analysis
- 10Be/9Be ratio measured by accelerator mass spectrometry
- Preliminary 9Be(n,g)10Be integral cross section results do not agree with current evaluated libraries

We are aiming to return to Oregon State University Jan- 2022 to perform the short time scale U238 irradiations

Reports with compendia of results for SLFPY

- "Interim Report on Fission Product Yields from the Irradiation of Np237 using the Godiva Critical Assembly", S. Burcher et al. Sept. 2020 LLNL-TR-1023214
- "Report on Short-Lived Fission Product Yields from Pu239", S. Padgett et al. LLNL-TR-799578 Dec 2019
- "Interim Report on Short-Lived Fission Product Yields from U238", J.T. Burke et al. LLNL-TR738508 Sept 2017
- "Interim Report on Short-Lived Fission Product Yields from U235", J.T. Burke et al. LLNL-TR704065 Sept 2016
- "Improved Cumulative Fission Yield Measurements with Fission Spectrum Neutrons on 235U," Nuclear Data Sheets, 155, 86–97, Jan. 2019, doi: 10.1016/j.nds.2019.01.005
- "Improved Cumulative Fission Yield Measurements with Fission Spectrum Neutrons on 238U," Nuclear Data Sheets, 163, 249–260, 2020, doi: 10.1016/j.nds.2019.12.006.

Cumulative Fission Product Yields and the R-Value

- An R-value is the ratio of the yield of a FP (i) to the yield of 99Mo (i = 99) in an unknown, relative to the same FP ratio from thermal fission (k =th) of 235U (j = 25).
- G.P. Ford and A.E. Norris, LA-6129 (1976)
- H.D. Selby, et al., Nucl Data Sheets 111, 2891 (2010)
- M.B. Chadwick, et al., Nucl Data Sheets 111, 2923 (2010)
- J. Laurec, et al., Nucl Data Sheets 111, 2965 (2010)

Execution

- Target preparation
  - Actinides for FPY measurements by:
    - Direct counting
    - Radiochemistry
  - Stacked foils for integral cross-section measurements in- and ex-core
- Irradiation at NCERC & Other (NNSS/DAF)
- Sample assay @ NCERC
  - LANL/LLNL counting facilities (HPGe coincidence)
- Sample shipping (from NNSS/DAF to labs)
  - Assay by gamma & beta
  - Post assay of list-mode data

Cumulative Fission Product Yield Sample Preparation

- Sample preparation (can involve more than one lab)
  - Select stock material and determine/verify chemical and isotopic composition
  - Actinides, e.g. 233U, 235U, 238U, 237Np, 239Pu, in 100s of milligram quantities
  - Geometric characterization of all target foils (mass and dimensions)
  - Sample containment prior to shipping (containment of Pu samples is part of the NPML)
- Sample shipping NCERC

- Current experimental activities involve multiple actinide (SNM) samples

Results For Experiments #4253 and 4256 (HEU)

- Comparison of current R-value results with R-values calculated from ENDF/B-VII.0 cumulative fission product yields for fission of 235U from 0.5 (fission) and 14 MeV neutrons.
- Difference, $\Delta R = R1 - R2$, between R-values determined from the high-power run (H) and those calculated for ENDF fission (*n* = ENDF) and from the low-power run (*n* = L).
- There is very good agreement between both data sets and ENDF for peak yield fission products, where we expect to see little fluctuation with incident neutron energy. However, differences can be seen in the valley and high mass wing

Results For Recent Experiments #4510 (PNNL DU), #4512 (LANL DU)

- Irradiation of DU at NCERC on Flattop in April 2021, samples split between LANL and PNNL.
- Comparison of R-values determined through whole A-solution or radiochemical separations performed by LANL and PNNL on a DU compared ENDF.V.III.0
- There is excellent agreement between the two laboratories and calculated ENDF values with some notable improvements to R-value uncertainties 10-1
    - 91Y, 136Cs

F**ission Chamber Performance**

- Pulse height spectra from the Mark II fission chamber
    - Benchtop testing with 252Cf
    - Testing at MIT with 235U
    - Both using P-10 fill gas

Conclusion

- Data from this and other projects will feed into a new FPY evaluation that will happen over the next few years.
- Regular interactions with another NA-22 funded multi-lab project "Evaluation of Energy Dependent Fission Product Yields"
    - LANL (leading lab) develops FPY models and produce the final FPY data files
    - BNL compiles experimental FPY data and produces a set of recommended FPY values, performs FPY data validation calculations
    - LBNL performs measurements of energy-integrated and differential CNAA (Cyclical Neutron Activation Analysis) using the intense neutron source by the LBNL cyclotron, and data interpretation by the FIER code
    - PNNL develops a new Bragg curve-based fission TPC (Time Projection Chamber) analysis in collaboration with LANL and LLNL
    - LLNL develops theories and methods to calculate primary fission fragment yields, and performs FREYA calculations for prompt decay

- The theory effort draws on the experimental results of several experimental activities funded by federal agencies through the Nuclear Data Interagency Working Group

FPY Data Compilations.
14:10 - 14:20
Dr Boris Pritychenko

EXFOR: Experimental Nuclear Reaction Data

- Manhattan Project alumni continued reaction compilations at Brookhaven in early 1950s.
- International cooperation in compilation areas #1, 2, 3 and 4 or NNDC, NEA-Databank Paris, NDS IAEA and IPPE, respectively, since 1969.
- Presently run by the Nuclear Reaction Data Centres (NRDC), internationally. This is an IAEA network which is coordinated by the IAEA.
- EXFOR team: B. Pritychenko (BNL), S. Hlavac, O. Gritzay, O. Schwerer (contractors), V. Zerkin (collaborator).
-

Missing Data in EXFOR
Not all experiments were compiled to SCISRS (Sigma Center Information Retrieval System, EXFOR precursor) database at Brookhaven in 1950s for historical (scope defined by applications) & technological (data were requested from authors or taken from published tables) reasons.
EXFOR project started to compile neuron cross sections and spontaneous fission since 1970, no FY until 1976.
Many important data sets were missed; comparison between EXFOR & Nuclear Science References (NSR) databases indicates that EXFOR could have 40,000+ experiments instead of 23,000.
Present day cost of a single experiment, LBL 88" Cyclotron example:

- $2,500 /hour beam time => $420 K/week
- Cost of 36S and 48Ca for ECR source are $47 K/gram and $250 K/gram, respectively
- Total price tag, conservatively, is $1 M
  It is cost effective to recover previous results than run new.

Missing FY data
NNDC is responsible for experimental nuclear reaction data in the Area #1.
Nuclear structure-like search for FY NSR references was conducted at NNDC, Fall 2017:

- Potentially Missing Neutron FY: 384
- Potentially Missing Spontaneous FY: 142
- Potentially Missing Photo FY: 126

Results were initially reported

- Informal NNDC-Los Alamos meeting, April 2018
- Workshop on Fission Product Yield Experimental Data, Los Alamos, August 20-23, 2018

- NRDC workshop, Vienna, October 22-25, 2018
- NRDC memos: CP-C 464, 465, 466, 469 (November 2018 – April 2019)

We analyzed the data, identified missing entries and collected PDFs (Not a trivial task but essential for compilations). **It took us 1 year to complete.**
The IAEA group started checking Mills, England & Rider for missing references in the Fall of 2018.
ND 2019 contributions, Beijing, May 19-24, 2019: NNDC & IAEA efforts.
Workshop on Fission Product Yield Experimental Data, Santa Fe, September 30 - October 3, 2019: NNDC & IAEA efforts.

Status of FPY Compilations

- Since 12/19/2019 the IAEA runs Updating Fission Yields Data for Applications CRP: https://www.iaea.org/projects/crp/f42007
- The CRP specific objective: Compile all available experimental data on independent and cumulative fission yields, measured total kinetic energies and total neutron yields, mass and charge-yield data.
- NRDC runs FY compilations worldwide in support of the CRP.
- NNDC finished four NRDC memos compilations by March 31, 2021.
- NNDC proactively finds and compiles other fission data.

NNDC Charged Particle FY Compilations

- Charged particles (p, d, t, 3,4He, ...) were extensively used to study FY at Berkeley, Los Alamos, Argonne, University of Washington, ...
- Many fissioning systems could be produced in charged particle reactions (Bohr-Independence Hypothesis):

• 232Th+4He->236U • 238U+4He->242Pu

- NSR contents were analyzed for charged particle fission reactions.
- NNDC raw compilation in FY2020 using NSR charged particle contents: 114 new and 7 updated.

Compiled all works of J. Wilhelmy (LANL) and G. Seaborg (LBNL)

Manhattan Project Data

- Fission yields and cross sections were produced by the Manhattan Project.
- Los Alamos National Laboratory library.
    - ~500 Los Alamos National Laboratory Reports were compiled into NSR database using the Primo library.
    - Nuclear reaction data reports from Los Alamos, Metallurgical and Pupin laboratories have been identified.
- Compilations of these data will start in December 2021.

Takeaways

- EXFOR FY compilation effort is complex and well-organized.
- Missing FY articles have been identified using NSR database (NNDC), R. Mills thesis and England & Rider (IAEA).

- NNDC (Area #1) finished four NRDC memos compilations and charged-particle FY by March 31, 2021.
- Further work will include extensive fission data search of the Manhattan Project lab reports to achieve completeness

FPY Evaluation Work at LANL
14:20 - 14:40
Amy Lovell

BeoH calculates prompt/delayed fission observables using the statistical Hauser-Feshbach theory
Both BeoH and CoH are deterministic Hasuer-Feshbach codes
Input from CoH is needed (fission probabilities, excitation energy, etc.)
The initial conditions of the fission fragments are parameterized and fit to data
Independent and cumulative mass yields show changes as energy increased
Cumulative fission product yields already show reasonable agreement without specific optimizations. This is good because there are often large gaps in the data

A Kalman filter has been used to further optimize the fission fragment initial conditions (first-chance fission)
The mass yields before neutron emission, Wahl scaling factors, total kinetic energy, excitation energy sharing, and spin cutoff parameter are included in the optimization
235U(n,f), 238U(n,f), 239Pu(n,f) prompt & delayed nubar, CFY for several isotopes
Okumura, Kawano, *et al*., arXiv:2102.01015 [nucl-th] 1 Feb 2021, in press JNST, LA-UR-21-20820

Description of the General Kalman filter provided. In essence, model parameter uncertainty developed using parameter sensitivity matrices and sandwich formula. Model predictions tuned to data

A variety of inputs are needed for BeoH calculations
Information on the compound nucleus – from CoH
Fission fragment initial conditions are parametrized (mass, charge, TKE, spin, parity distributions) and taken as free parameters in the FPY optimization
Model parameters are updated with uncertainties and
correlations
Prompt and delayed neutron multiplicities are reproduced simultaneously
A variety of cumulative fission product yields can also be reproduced, both mean and covariance

A stepped approach is being used to include the bulk of the experimental data into the optimization

1) including a handful of important-to-model nuclei, 2) nuclei with good energy dependence [up to Einc=5 MeV], 3) light nuclei, 4) heavy nuclei

Many FPYs show reasonable agreement with experimental data for light and heavy nuclei
Prior may be off, but get fixed in adjustment

Non-linearities in the model can lead to significant differences between the Kalman and BeoH posteriors
The majority of FPYs match reasonably well between Kalman and BeoH (linear assumption is okay), but BeoH may still not describe data

Differences between Kalman and BeoH could be mitigated through several means
Potential challenges:

- Calculations are not run with a low enough Y(A,Z) threshold: missing contributions to cumulative yields and sensitivities
- Sensitivities are EXTREMELY non-linear and should be calculated much closer to the best fit parameter set
- Small uncertainties on the data pull to hard on the optimization (FPY templates exist, Neudecker, et al., LA-UR-19-31156)

Ultimately, we may have to put a correction on top of the BeoH calculations to ensure we reproduce important FPYs.

Correlations between cumulative (and independent) fission product yields can be calculated

The Kalman filter can be further be extended to include the energy-dependent parameters
Giving us access to correlations between FPYs and across energies

Summary

- The Hauser-Feshbach fission fragment decay code, BeoH is being used to consistently calculate independent and cumulative fission product yields, simultaneously with other prompt and delayed observables.
- A Kalman filter has been implemented to adjust parameters describing the fission fragment initial conditions to prompt and delayed average neutron multiplicity and certain thermal cumulative fission product yields with low reported uncertainty in the England and Rider evaluation, for first-chance fission (up to 5 MeV).
- First-chance fission for 239Pu is currently being studied in detail to include the bulk of the experimental cumulative FPY data in the optimization. Discrepancies between Kalman, BeoH, and data need to be addressed either through modeling or additional corrections. Methods will be extended beyond first-chance fission.
- Covariance across the FPYs are being constructed (more during covariance session).

- 235U, 238U, and 239Pu for first-chance fission are in good shape; initial calculations for 252Cf have been started, and input for 237Np is being prepared.

Angular Momentum Studies with FREYA
14:40 - 15:00
Ramona Vogt

Recent experimental information on spin correlations

- Angular momentum generation in nuclear fission, J. N. Wilson *et al.,* Nature 590 (2021) 566
- OBSERVATION: ``*There is no significant correlation between the spins of the fragments''*
- INTERPRETATION: *Therefore ``the fragment spins are generated after the nucleus splits'', i.e. ``after the fragments have become two separate, independent systems''*

Mechanism of fragment spin generation: Nucleon exchange in the dinucleus

- Relevant theory of nucleon exchange *Damped heavy-ion collisions,* W.U. Schröder and J.R. Huizenga, Ann. Rev. Nucl. Sci. (1977) 465
    - Intimate relationship between nucleon exchange and energy dissipation
- *Theory of transfer-induced transport in nuclear collisions,* J. Randrup, Nucl. Phys. A327 (1979) 490:
    - Each transfer changes the nucleon numbers and the excitation energies of the fragments, as well as their linear & angular momenta
- *Transport of angular momentum in damped nuclear reactions,* J. Randrup, Nucl. Phys. A383 (1982) 468:
    - Mobility (friction) tensor: anisotropic
- *Dynamical evolution of angular momentum in damped nuclear react*ions, T. Døssing and J. Randrup, Nucl. Phys. A433 (1985) 215:
    - Relaxation times: $t_{\text{wriggling}} << t_{\text{bending}}$ & $t_{\text{twisting}} <<< t_{\text{tilting}}$

Normal rotational modes of a dinucleus at scission

- Studies in the liquid-drop theory of nuclear fission, J.R. Nix and W.J. Swiatecki, NP 71 (1965) 1

Diagonalization of the rotational energy in fission

- All rotational modes of the dinucleus are assumed to be in thermal equilibrium
- *Equilibrium statistical treatment of angular momenta associated with collective modes in fission and heavy-ion reactions,* L. G. Moretto and R. P. Schmitt, Phys, Rev. C 21 (1980) 204 :

Angular momentum
Shapes considered
conservation leaves six independent rotational mode

In FREYA: The fragment spins are determined at scission
Fragment angular momenta are correlated due to normal modes but are nearly independent nonetheless
Dominance of fluctuations results in very weak fragment spin correlation
Even highly correlated contributions can result in uncorrelated results – can be calculated & published several papers on them: JR & RV, PRL 127 (2021) 062502, RV & JR, PRC 103 (2021) 014610

Wilson et al. also measured fragment spins:
Measured S(A) is sawtooth-like,
similar to n(A), and, possibly, ng(A) although new measurements should be made to confirm this behavior

We can model S(A) of the fragments & compare to data
Default moments of Inertia in FREYA have a simple dependence on mass:
$I_L \sim (1/2) M_L R_L^2$ $I_H \sim (1/2) M_H R_H^2$
This simple dependence means that S(A) has a weak dependence on A
If the default moments of inertia are replaced by moments of inertia that schematically depend on the ground state deformation of the fragments, get better description of experimental data.

Modeling of moments of inertia reinforced by microscopic models
Spin distributions calculated recently in microscopic models
P. Marevic, N. Schunck, J. Randrup and R. Vogt, PRCL 021601 (2021) – Editor's Suggestion
Spin distribution fitted by:

$$|a_J|^2 \propto (2J + 1) \exp[-J(J+1)/2s^2]$$

Where s^2 = I, the spin cut-off
Parameter proportional to the moment of inertia
However, I is the moment of inertia at scission

- Analytical formulas are rough approximations
- Deformation at scission could be very different than in the ground state

Angular Momentum Projection Allows Us to Calculate S(A) in Microscopic Models
First-ever microscopic prediction of spin distributions across a broad range of Fragmentations, used to simulate γ emission in FREYA: good agreement with Wilson et al (albeit for 239Pu(n,f))
• Extract spin distribution from HFB solutions by angular momentum projection

Fission yields interplay with beta-delayed neutrons and electrons
15:00 - 15:20
Dr Alejandro Sonzogni

Beta-delayed neutron activity
ENDF uses 6 while JEFF uses 8
In U235
The halflives are different in ENDF, but identical in JEFF
Delayed neutron multiplicity is sum of exponentials
Divided by Keepin 6-exp fitting to precisely measured activities. Up to 20% diff between Keepin and JEFF
Issue raised by INL and ORNL
The longest lived group corresponds to 87Br with T1/2-56.65 s, a=CFY*Pn, which is well known
Delayed nubars unchanged, so do not explain difference

Similar for 238,233U

Probabilities and spectra for each group are given in MT-5, MF-455. Based on Brady and England

Showed spectrum as a function of time. At t=40 s, see 30-40% diff between ENDF and JEFF between 235U. For 239Pu, JEFF and ENDFB7.1, see mostly agreement

Argue to redo MT=1,5 MF455 for ENDF/B-VIII.1. Project will build on IAEA CRP on beta-delayed neutron emission, published in NDS. For minor actinides, can use FY & decay data are in much better shape now. Estimate will take 2-3 years

Beta-delayed electrons
Measurements of gamma and beta spectra by Kirk Dickens and collab. In 1970's from ORNL to quantify decay heat in LOCA reactor scenario. Cor irradiation with rabbit system. 1-10micrgram foils. # fission determined from ^{97}Nb, ^{99}Mo, ^{231}Te gammas, 1.5% uncertainty

Electron spectra measured HOW

Compared to calculations using ENDF/B-VIII.1 decay data, good agreement for 235U at 1sec. For 239Pu, agreement worse, esp. at high energy. To improve fit, need to consider IFY

For 241Pu, does great

From Dickens, backed out antineutrino spectrum in equilibrium and very good agreement with current simulations, with no reactor anomaly. Comparision of ratios of ORNL, ILL and 2021 measurement shown

Session: Evaluation Committee - Charged Particles

Summary of the light-element CP induced evaluations for VIII.1
15:20 - 15:40
Dr Mark Paris

- Tapes–all extended energy/better agreement with more data; Covariances planned
  - p-001_H_001.endf
  - p-002_He_004.endf - extend upper energy from 20 MeV to 34 MeV
  - d-002_H_003.endf – extend upper energy from 1.4 MeV to 20 MeV
  - d-002_He_003.endf
  - d-003_Li_006.endf
  - t-002_He_004.endf - higher energies, more channels (esp. inelastic-like reactions)
  - a-006_C_013.endf
- Testing
  - NJOY
  - IAEA/Dunford codes [checkr, stanef, fizcon, psyche, inter]
  - ENDF>ACE
    - checkace [LANL ACE format checking tool]
    - mcnp6.1 pencil beam (d+3He only)
- Comparisons
  - with ENDF/B-VII.1 (*aka*, "CP2011"), VIII.0
  - with LLNL *Evaluated Charged Particle Library (ECPL-2018)*

17O system- significant progress

- # channels: 45 • J$\boldsymbol{\pi}$=1/2±, ..., 11/2±
- # parameters • Eλ: 81 level energies • $\gamma\lambda$,c: 322 reduced widths
- # Normalizations • n : 95 norm scales M • ΔEM: 4 shift factors

Lot of work went into 13C(a,n0) and 12C(a,n1)

MF=6 required for CP data, but there is no mechanism to provide covariances in ENDF format for MF=6. Can do it with MF=30 parameter covariance, but no one knows how to process this (nor even how to pack it)

What is to be done

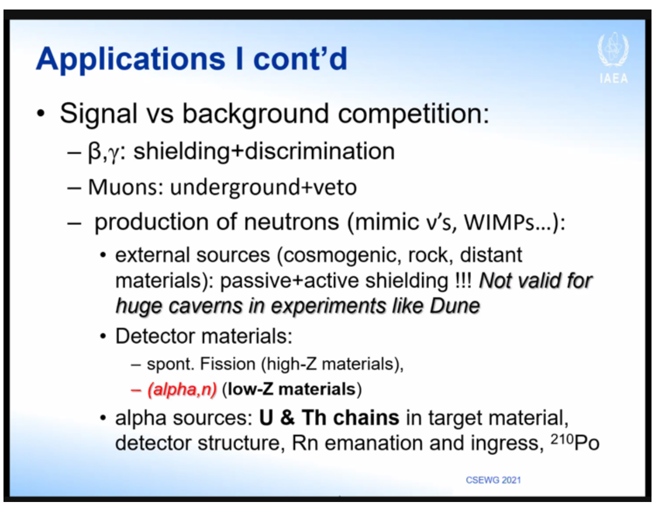
- p-001_H_001.endf
  - extension to 100 MeV of multichannel evaluation
  - punch MF=2 LRF=7 (KRL=1) sections
  - generate covariance sections
- p-002_He_004.endf
- d-002_He_003.endf

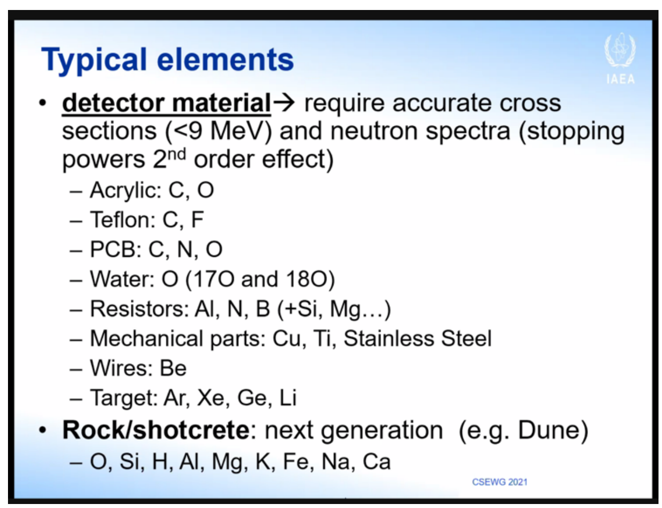
- d-003_Li_006.endf
    - 6Li(d,n) now to 20 MeV
    - need to include angular distribution data
- t-002_He_004.endf
    - cross sections complete for all of the above
    - punch MF=2 LRF=7 (KRL=1) sections
    - covariance file generation needed
- a-006_C_013.endf
    - complete the 17O system evaluation (~ 2 months)
    - punch ENDF files (ENDFtk)
        - MF = 2,3,6,32,33

TM on (alpha, n) nuclear data evaluation and data needs
15:40 - 16:00
Paraskevi Dimitriou

Review measurements, needs and evals and on-going projects

61 registrants
Low-background rare events, nucl. Astro., fusion, nonprolif





Nuclear astrophysics
Various experiments at LUNA, Notre Dame, Ohio U. NTIF, TAMU, TRIUMF
S process: 13C(a,n), 22Ne(a,n), 17O(a,n), 17O(a,g)

Fusion – account for alpha loss, lose energy of plasma. Anuetronics, activation foils. Need (a,n) library of cross sections so can do scoping study

Non-proliferation: UF6 enrich, spent fuel, passive NDA, source characterization)
Sources4c, C. Romano, need F, O, C (a,n)
Strong overlap with other application needs

Reactor operations & safeguards
Core calc. & neutron leakage
Dedicated session on 17O session
New evaluations from Chen-Tsinghua U, LANL
New measurements from GELINA, Ohio U, Notre Dame and IPPE
None of new data considered in new evaluations yet

Also new a+9Be from CEA Cadarache

New applications being developed
Sources4a (Sheffield)
Neubot (MIT
SAG4N

R-matrix models need extension (Faddeev, breakup, higher energies). Also (HF ingredients)

INDEN-light element working group
N+9Be, n+14,15N, n+16O, n+23Na

Thursday 18 November 2021

Session: Evaluation Committee - Neutron sublibrary

Current status of ENDF
10:00 - 10:30
Dr Gustavo Nobre

Topics:
- GitLab: git.nndc.bnl.gov

- Meetings since last Nuclear Data Week: mini-CSEWG
- Next ENDF Release
- Updates in the ENDF library since last Nuclear Data Week
- Main challenges to be addressed

2020 minutes are available (https://indico.bnl.gov/event/7233/page/354-csewg-minutes) as are the mini-CSEWG minutes (https://indico.bnl.gov/event/12258/attachments/35490/61392/mini-csewg-mini-minutes-final.pdf)

Gitlab is working:

- Many issues are being found and logged as issue trackers
- Some have been fixed, many are still there (Hackaton?)
- Contributions are being sent and uploaded in appropriate Phase 1 branches (or separate branch if conflicting)

Mini-CSEWG report

- Virtual
- DOE/SC PuRe initiative and ENDF implications
- Contributions for neutron, TSL, CP & photonuclear sublibraries
- Evaluation review
- Validation
- Discussion and poll: To adjust or not to adjust?

Evaluation reviews are finally working, Gustavo will be assigning reviewers

To adjust or not to adjust: we voted NO (for now)

Next ENDF release will be postponed 1 year, to Feb. 2024

- COVID pandemic delayed many experiments: New data are expected
- Need more time to setup proper review process
- Not enough time for proper testing and validation
- Time deal with a potentially serious issue at high reactor burn-up

Updates to the ENDF library since last NDW:

- TSL: 18 (NCSU), 9 (NNL), 7 (JEFF), 7 (RPI), 3 (LANL)
- neutrons: 56Fe (IRSN), 86Kr (BNL), 29 files (RQW+BNL), 103Rh (RPI), Cd (LANL), 235,238U (INDEN)

Burnup Issue:

- Calculations with VERA benchmark found a loss of reactivity at high burnup, which discouraged adoption of VIII.0 by the nuclear reactor community.
- There are leads:

- At the IAEA INDEN meeting, it was likely tracked down to a modest change in the 238U(n,g) cross section in ENDF/B-VIII.0
- The change may be correct. However, in the transition to VIII.0, 239Pu was not updated
- Athighburnup,238Ubreeds239Puandthis compensates for the burning of 235U
- Other issues need to be clarified

Conflicting evaluations and the TSL contributions:

- ^{56}Fe:
  - INDEN solves leakage issue
  - IRSN: extend R-matrix to inelastic channel
- TSL (graphite, lucite...)
- TSL library is expanding:
  - VI.8 had 15 TSL materials
  - TSL was unchanged from VII.0 to VII.1 (20 materials)
  - 14 TSL evaluations updated in VIII.0 (totaling 24 materials)
  - Library will be extended to ~30 materials in VIII.1
  - Ran out of MAT numbers: Approved format change to solve this

Gamma spectra:

- Many strong disagreements between ENDF and ENSDF
- Worse agreement with data when transitioned from VI.8 (elemental) to VII.0 (isotopic)
- Quality of gamma spectra needs to be recovered (many, many applications!)
- ^{55}Mn INDEN evaluation showed a path to address these issues
- GRIN proposal is funded!!

Status of isotopes, covariances, review process, other future work

- ^{239}Pu (Marco, Roberto)
- ^{181}Ta (M. Herman)
- Cu (T. Kawano, LANL)
- Planned Zr: ORNL + BNL
- Some neutron contributions still lack covariances

We plan to go full-speed soon on the review process through GitLab. We will sketch out the future Big Paper so no evaluation left behind!

Solving the burnup conundrum: Updates in U-235 and U-238 evaluations in the RRR
10:30 - 11:00
Andrej Trkov
Marco Pigni
Roberto Capote

Loss of reactivity with burnup for PWR with ENDF/B-VIII.0 library compared to ENDF/B-VII.1

- Reported by Kang Seong Kim et al. at CSEWG 2019
- Extensive analysis by Kang Seong Kim and William A. Wieselquist in J.Nucl.Eng. 2021,2, pinpointing the problem to U-238
    - Criticality prediction of U-238 was benchmarked extensively – small differences overall
    - Problems appear with burnup:
        - FP yields library unchanged from ENDF/B-VII.1
        - Major FP cross section not so different
        - Focus on Pu-239 production

Differences in reactivity when individual nuclides from ENDF/B-VIII.0 library are substituted into ENDF/B-VII.1 (K.S. Kim et al., J.Nucl.Eng. 2021,2, Fig.2)

INDEN update of U-235 evaluation (ORNL/IAEA/JSI):

- Detailed fission-XS shape that follows better the fluctuating data in the URR
- Spurious cross-reaction covariance elements between the resonance and the fast energy ranges removed to avoid negative eigenvalues.
- Cross-covariances between nu-bar and fission cross section removed for the same reason.
- RRR: additional work below 20eV to improve agreement with RPI data
- See INDC(NDS)-0810, IAEA INDEN-ACT III meeting: capture decreased from 0.0623 up to 11eV
- U-235 file: nds.iaea.org/INDEN/data/u235ib46o28t6DNcnu5ef0STzt_ENDF.zip

What is different in ENDF/B-VIII.0 ?

- U-238 in ENDF/B-VIII.0 is a CIELO evaluation (R. Capote, A.Trkov et al., Nucl.Data Sheets 148 (2018) 254-292)
- Thermal reactors → let us focus on the lower resonance range
- Slight change was made in ENDF/B-VIII.0 to the bound level widths to fit the measured transmission data of Olsen.
- This affected the capture below and above the first resonance by about 2–5%.
- Thermal value was unchanged.

Cumulative U-238 capture reaction rate integral in a PWR spectrum:

- Thermal part of the spectrum in a PWR is suppressed due to boron in the coolant, emphasizing the importance of the epithermal energy range.
- Importance of the resonance range up to 200eV emphasized by D. Bernard and O. Cabellos at the INDEN IAEA TM (Nov. 2021)
- Cumulative reaction rate integral ratio of U-238 capture (at infinite dilution) between ENDF/B-VIII.0 (label "e80") and "e80V02" (with resolved resonance data substituted from ENDF/B-VII.1) increases up to ~200 eV, except at the 6 eV resonance.

- The opposite effect of the 6 eV resonance diminishes when self-shielding is taken into account

Data substitution exercise:

- Replace resolved resonance parameters in ENDF/B-VIII.0 by ENDF/B-VII.1, keep background in (n,f) (filename “u238e80V02b”)
- Process with NJOY into WIMS-D format
- Replace U-238 in the WIMS-D library with “u238e80V02b”
- Supercell calculations with WIMSD-5B
- Test enrichments 2.1% and 4.75% at HFP conditions

Reactivity trends due to ^{235}U, ^{238}U (k_inf of central cell)

- Enrichment 2.1%
  - Reactivity starts low at -200 pcm and increases
  - After a few 1000 MWd/tU becomes steady at about +150 pcm
- Enrichment 4.75%
  - Reactivity starts low ~150 pcm and increases steadily
- Compared to ENDF/B-VIII.0, updated files produce reactivity trends closer to ENDF/B-VII.1

Why WIMS-D ?

- Full control of the library
- Runs quickly
- We are only interested in relative differences
- We already have a library based on ENDF/B-VIII.0
- WIMS-D calculations were benchmarked with Serpent and OpenMC on ENDF/B-VIII.0 data

Pu-239 buildup

- Enrichment 2.1%
  - Pu-239 continues to increase at high burnup
  - The increase partly compensates reactivity loss
- Enrichment 4.75%
  - Pu-239 reaches saturation
  - Its steady concentration does not compensate reactivity loss

Conclusions

- Resonance substitution in U-238 from ENDF/B-VII.1 into ENDF/B-VIII.0 indeed compensates large reactivity loss of with burnup; small contribution comes from U-235
- The higher capture in the energy region 0.1 – 100 eV in ENDF/B-VII.1 decreases initial reactivity, but enhances Pu-239 production

- The Pu-239 production at 4.75% enrichment leads to saturation, while at 2.1% enrichment Pu-239 concentration continues to increase → the trend of reactivity loss is stronger at higher enrichments
- New U-238 RRR evaluation desirable
- Possible solution is offered at: nds.iaea.org/INDEN (U-238 tab, v02b)

INDEN evaluation of n + (U-233), Pu-239: status and updates
11:10 - 11:40
Roberto Capote

Outlook

- Thermal Neutron Constants (standards)
- PFNS
- U-233 short review
- Pu-239 status
- Planned updates

Thermal Neutron Constants (STD 2017)

- B8 235U(nth, f) fixed, 239Pu(nth,f) still low, 241Pu(nth,f) still low

Developing new integral contraints for RP fit to fissile targets

- All measured ToF high-resolution data (1955-2019) used to derive:
    - I_1, I_3, I_3/I_1, $\sigma_f(th)/I_1$
- May require small revision of RP fits for all fissiles
- Duran et al. (2021) discussed at INDEN CM Nov. 2021

n_{th}+X PFNS <E> (IAEA 2016, STD 2017)

- ENDF/B-VIII.1 candidate evaluations
    - Pu-239: LANL new evaluation based on ChiNu + CEA data ready + IAEA thermal
    - U-235: LANL new evaluation based on ChiNu (almost) ready + IAEA thermal
    - U-233: IAEA thermal + Talou, Rising 2016 evaluation
- ALL RPs were refitted, nubar(E) !!!
- ORNL in collaboration with IAEA/JSI

INDEN updated "actinide" evaluations

- ^{233}U (ORNL/IAEA/JSI) nds.iaea.org/INDEN/data/u233a506b-c_ENDF.zip
    - PFNS: Use of the IAEA U-233(n_{th},f) PFNS <E>=2.030 MeV vs ENDF/B-VIII.0 <E>=2.074 MeV). Talou et al PFNS evaluation (IAEA PFNS CRP) is used in the fast region.
    - Adjustment of thermal cross sections to agree with TNC from IAEA Standards 2017 (=B8).

- Introduction of energy dependence for nubar below 30eV from Reed et al data.
    - RRR refitted at ORNL (see Pigni's talk).
    - ENDF/B-VIII.0 adopted JENDL-4 fast neutron region based on the paper: Nuclear Data Sheets 139 (2017) 138–170
    - Fast neutron nubar needed minor changes to compensate loss of criticality due to softer PFNS by Talou et al (see NDS PFNS paper)
    - BIG improvement in performance of U-233 solutions ! Good k_{eff} vs ATLF trend (PFNS thermal + new resonance parameters)
- ^{239}Pu RRR to be discussed by M. Pigni
    - Status of INDEN Pu-239 evaluation: RRR - Presented by M. Pigni at IAEA INDEN-AC 2020, CSWEG 2020

^{239}Pu RTC-MISTRAL2 experiment, CEA

- Modifications to the RR fit required:
    - ↑subthermal α, ↓ α till 1eV (closer to B8)
    - To improve RTC and ↑ crit. @ high burnup
- NOTE: ↑ crit. may compensate U-238 criticality reduction

Comparison plot of EMPIRE (p27) vs ENDF/B-VIII.0 for 239Pu was shown

Criticality validation (main fast benchmarks)

- 235U same;
- U-233 need small nubar tweak (increase)
- 239Pu INDEN03 (p29,p35,p38) good

LPS validation (currently better than B8)

INDEN updated "actinide" evaluations

- Pu-239 (ORNL/IAEA/JSI), current EMPIRE (p27)
    - <u>Validation of this file already presented</u> in Denise's 2021 talk
    - Updated standards with NIFFTE data + UQ
    - Fission term: LANL nubar evaluation + PFNS fast, IAEA PFNS th
    - RRR refitted at ORNL/IAEA/JSI (see Pigni's 2020 talk)
- **<u>To do:</u>**
    - Use of Mosby data to improve capture (slightly lower capture may be needed)
    - Reevaluation of nubar(E) in 1-80keV using Gwin data
    - Reevaluation of nubar considering (n,gf) data
    - Addressing reactivity temperature coefficient issue: Increase of subthermal alpha/ Decrease of alpha above thermal and below the first resonance)
    - Study of impact of changes in the low-energy RRR on burnup
- **<u>Further improvement:</u>**
    - Soft-rotor model (SRM) optical model potential - even better physics for neutron scattering description.

- ^{239}Pu(n,γ): ENDF/B-VIII.0 vs Mosby data - Mosby data is slightly lower from 10 – 200 keV

Future Updates:

- Optical model for soft deformed nuclei:
  - Conventional OMP
    - Soft spherical nucleus (vibrational excitations)
    - Rigid deformed nucleus (rotational excitations)
  - Actinides: Big static deformation – **expansion around statically deformed shape**
  - E.S. Soukhovitskii, RC et al, PRC94(2016)064605, erratum: PRC102(2020)059901
  - DCCOMP based on Soft Rotator Model (SRM) for deformed nuclei

^{239}Pu(n,inl): SRM vs Rigid OMP

- Criticality increase in SRM vs. p27 compensates for (n,g) reduction

^{233}U coupling scheme: New OMP 2420

- Octupole band (on $5/2^-$ state) and β-band (on $5/2^+$ state) coupled
- Octupolar: $5/2^- \equiv$ (core exc) $0^- \otimes 5/2^+$ (single-particle GS)
- Quadrupolar: $5/2^+ \equiv$ (core exc) $0^+ \otimes 5/2^+$ (single-particle GS) better physics lead to better nuclear data

INDEN Summary

Updated evaluations of major actinides available from INDEN

- See Andrej Trkov talk:
  - U-238 (nds.iaea.org/INDEN/data/u238e80V02_ENDF.zip)
  - U-235 (nds.iaea.org/INDEN/data/u235ib46o28t6DNcnu5ef0STzt_ENDF.zip)
- In this talk:
  - U-233 (nds.iaea.org/INDEN/data/u233a506b-c_ENDF.zip)
  - Pu-239 (nds.iaea.org/INDEN/data/pu239e80p38_ENDF.zip = p39) see validation in Denise talk
- Future updates planned
  - U-233: Nubar tweaks for fast neutrons needed (+ 0.1-0.2% ~ 0.5σ)
  - Pu-239: RP fit needs minor modifications below 2eV (RTC, ref. integrals, TNC)
  - Pu-239: Drop ENDF/B-VIII.0 Pu-239(n,g) capture to better reproduce Mosby data
  - Pu-239: New SRM optical model to be used for even better inelastic scattering
- The **INDEN** scheme of international collaboration **is working well**.

Structure in 239Pu capture != structure in fission

URR for 233,235U and 239Pu

11:40 - 12:10

Dr Marco Pigni

Evaluated data for fissile actinides in the Resolved and Unresolved Resonance Region and their coupling to neutron multiplicities

Presented at INDEN meeting a week ago

Overivew

- 233U
  - Motivation: underestimated reactivity for critical assemblies
  - Status: updates to PFNS, thermal constants, R-matrix improved subset of benchmarks [1]
  - RRR: extension up to 2 keV and inclusion of possible newly measured capture data
  - URR: relevant to assess impact on benchmark calculations in the energy range 2–40 keV
- 235U
  - Motivation: investigation on reactivity rates related to depletion calculations
  - Status: 238U evaluation (see Capote/Trkov presentation) affecting the burn-up trend
  - URR: updated evaluation by including recently measured fission data
- 239Pu
  - Motivation: R-matrix analysis to include TNC values (STD 2017) and PFNS (IAEA+LANL)
  - Status: partial work to extend RRR up to 5 keV
  - Neutron multiplicities: updated evaluation with fluctuations and related covariances in progress

[1] Annals Nuclear Energy 163 (2021) 108595.

Focus on URR in 235U

- Preliminary SAMMY/FITACS fit of available total, fission, and capture data sets. Elastic channel computed by difference and inelastic channel parameterized by neutron strength functions and energy scaled penetrability factors.
- Except for inelastic channel (11%) scaling factors ranging up to 6%
- Except for fluctuations, reasonable agreement with B8
- 20 keV is acceptable upper energy limit for URR fit to account for self shielding effects
- ENDF/B-VIII.0 evaluated data show fluctuating behavior (to be checked if there is formal consistency between file 2 and file 3)
- Inelastic channel deviates from B8 below ~10 keV
- Difference is in microbarns, so harmless
- Next step is the inclusion of fluctuations! (Resonance parameters ⇒ fit ⇒ effective/theoretical cross sections): How to include fluctuations cross sections?

239Pu neutron multiplicities with fluctuations and related covariances in progress
(n,g+f)

- Fluctuation behavior of prompt neutrons based on competition between (n,g+f) and (n,f)
- Resonance fission widths for each level used to calculate the partial energy dependent fission cross section

Neutron multiplicity of 239Pu

- Measured data with different resolution. Ryabov seems the most consistent
- As expected the correlation matrix reflects the nubar fluctuation behavior
- To reduce size of covariance matrix, energy grid properly defined around each energy level
- Calculated uncertainty is about ~0.3%

239Pu evaluation updates in the fast energy range

12:55 - 13:25

Denise Neudecker

Matthew Mumpower

SUMMARY OF CURRENT STATUS: UPDATES SINCE ENDF/B-VIII.0:

- We are in the process of updating the ^{239}Pu cross sections in the fast energy range (complementing the work of IAEA / INDEN / ORNL lower energy work in the resonance range)
- LANL has been overhauling its evaluation tools (CoH, CGMF, DeCE, Kalman, NEXUS, PySOK, SOK)
- Focus on consistency throughout evaluation (we are evaluating more isotopes)
- Model update: new collective enhancement allows for simultaneous description of (n,f) and (n,2n) channels
- Model update: new inelastic scattering model using the Engelbrecht-Weidenmuller transformation
- New cross section evaluation goes up to 30 MeV (as well as nu-bar and PFNS)
- New (n,g) data from S. Mosby up to ~1 MeV
- Neutron Data standards ^{239}Pu(n,f) cross section; includes updates in covariances with templates and new (n,f) data from fissionTPC (Snyder)
- New nu-bar including improved exp. UQ, Marini data and consistent CGMF modeling
- New PFNS: INDEN non-model evaluation at thermal, Los Alamos model evaluation above including new Chi-Nu and CEA data
- We are actively testing the file versus integral benchmarks; starting covariances

TOTAL CROSS SECTION:

- Model: Soukhovitskii (2005) optical model [deformation ~0.21]; coupled channels with 7 levels

- Tuned parameters using Bayesian Hyperparameter Optimization to fit to ENDF/B-VIII.0 and parsed EXFOR compilation
- We fit the Soukhovitskii (2005) optical model parameters (potential depths, radii and diffuseness)
- Soukhovitskii (2005) also depends on deformation, but it is not well constrained given cross section data
- A cautionary tale; higher dimensional spaces are tricky; holding fixed some parameters is necessary

Capture Cross Section:

- Model: M1 enhancement employed from systematics of Mumpower et al. PRC 96 024612 (2017)
- New cross section data incorporated from S. Mosby et al. NDS 148 312 (2018)
- ENDF/B-VIII.0 has some oscillatory behavior around 10 keV
- The LANL CoH model in contrast is rather smooth; in agreement with Mosby data

(n,2n) cross section:

- Model: new collective enhancement allows for simultaneous description of (n,f) and (n,2n) channels [difficult to describe in past versions of CoH]
- Tight integration of model and experimental data leads to the updates relative to ENDF/B-VIII.0
- we are actively testing this change

ELASTIC CROSS SECTION:

- Model: generally tracks ENDF/B-VIII.0 with more substantial differences above 10 MeV
- Note that there is a large spread in evaluations as compared to other channels

INELASTIC CROSS SECTION:

- Model: new inelastic scattering model using the Engelbrecht-Weidenmuller transformation (collective enhancement → removal of fictitious levels); similar to IAEA results
- At higher energies we're higher than other evaluations, which could be increasing criticality for fast assemblies. New tests needed with pulsed spheres. With EW transformations leading to collective enhancement
- Again, a large spread in evaluations as compared to other channels
- Threshold behavior is similar to ENDF/B-VIII.0 [logscale between 5 keV and 5 MeV]

Elastic cross section at 3 degrees performs similar to ENDF/B-VIII.0.

Inelastic cross section data of Smith et al., (1982) constrained by level energy. Performs similar to ENDF/B-VIII.0; Excitation energy between 0.08 and 0.3 MeV; energy resolution not quoted.

Elastic plus inelastic angular distribution: Performs similar to ENDF/B-VIII.0; Incident neutron energy 2.5 MeV; 7 levels under 200 keV quoted 3% exp. Uncertainty. We seem to perform slightly better than ENDF/B-VIII.0 @ 14 MeV; Kammerdiener energy resolution ~1 MeV. Collective enhancement should improve Eout = ~8-9 MeV region

Fission cross section: This evaluation differs from the VIII.0(n,f) crsoss section; it comes out of standards analysis including updated covariances using the template approach and fission TPC data; it is a reference cross section. Our evaluation goes up to 30 MeV (part of the Iaea standards effort). Pu239 is not a standard, it is a reference.

- Cross sections in the fast range are similar to VIII.0
- High-precision data by fissionTPC (used as shape) confirms overall trend of fission-chamber measurements
- Standards are discussing the normalization factor published by fissionTPC data and how it relates to spectral indices in LANL fast critical assemblies

Prompt nu-bar:

- Requires small additional tweak since presentation at mini-CSEWG (2021) improving keff performance.
- Nu-bar includes CGMF modeling, Marini data (measured with Chi-Nu array) and better experimental UQ. Marini data confirmed VIII.0 between 0.8 and 2 MeV

Our current evaluation is higher than VIII.0 below 0.8 MeV because two data sets were rejected for physical reasons
Tweaked evaluation between 100keV and 1 MeV to get better results for Jezebel

Adopted INDEN PFNS:

- No changed since mini-CSEWG (2021).
- PFNS includes high precision Chi

Validation:

- Ongoing
- LANL has a problem with pulsed sphere, it is being fixed now

^{235,238}U PFNS and (n,f) cross section:

- Work is ongoing as part of the Neutron Data Standards effort to update covariances of past experimental data related to ^{235,238}U(n,f) cross sections in GMA
- ^{238}U(n,f) cross sections could be included in ENDF/B-VIII.1
- ^{235}U PFNS: work is currently ongoing to include new Chi-Nu data, work by A. Lovell, D. Neudecker & P. Talou also underway to model via CGMF (challenging)
- Cannot update U5 because that's standard and would delay release
- 238U PFNS: Chi-Nu data scheduled to be coming shortly before the release of ENDF/B-VIII.1

Working towards update of 235U(n,f)nubar_p (Experimental data only)

- Started evaluation from scratch (no input files from Phil Young found), uncertainties of experimental data were reestimated using templates of expected uncertainties
- New data since last ENDF/B evaluation: Boikov and Khoklov, Khoklov data pull evaluation down below 1 MeV
- 2nd chance fission threshold more clearly observed
- Evaluated uncertainties were increased compared to VIII.0 to account for newest standard uncertainties
- Including CGMF modeling (A. Lovell is doing the modeling)
- Below 1 MeV: We are just exploring if there should be a bend in <TKE>
- Evaluated uncertainties increased compared to VIII.0 to account for newest standard uncertainties

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- New PFNS: INDEN non-model evaluation at thermal, Los Alamos model evaluation above including new Chi-Nu and CEA data
- We are actively testing the file versus integral benchmarks; starting covariances

Comments from after the presentation: Roberto Capote warned about varying OMP parameters too far, leading to miss information from the good fits obtained for BOTH neutron and proton reactions.

239Pu evaluation
13:25 - 13:55
Gregory Potel Aguilar

Presenter could not attend CSEWG

TN update plans and advances for 16O and 9Be
13:55 - 14:25
Dr Mark Paris

TN = thermo nuclear

Outline
- Thermonuclear/charged-particle evaluation updates
- n+9Be status & plans
- n+16O progress report

Thermonuclear/charged-particle reactions
- Detailed in earlier Charged-particle session 2021-11-17
- Evaluation updates & new evaluations
    - p-001_H_001.endf
    - p-002_He_004.endf
    - d-001_H_003.endf
    - d-002_He_003.endf
    - d-003_Li_006.endf
    - t-002_He_004.endf
    - a-006_C_013.endf

n+9Be evaluation
- Light-element R-matrix evaluation R-matrix formalism
- EDA R-matrix evaluation procedure
- Added data: elastic, (n,α), (n,n_1)
- Integrated Cross Sections plots shown:
    - n+9 Be Total Cross Section,
    - 9 Be(n,α) 6 He Cross Section,
    - 9 Be(n,n)9 Be Cross Section,
    - 9 Be(n,2n)αα Cross Section,
    - all with good agreement with data
- Elastic differential CS (angular distributions) were also shown with good agreement with data

Summary of new evaluation:

- 10Be analysis has produced a consistent set of cross sections and angular distributions that are in agreement with most of the experimental data at energies up to 5 MeV. Extensions above that energy were based on the experimental data alone.
- Level assignments for the overlapping resonances near En=2.7 MeV have the opposite parity (4- ,3+ → 4+,3-).
- Excited states of 9Be make important contributions to the (n,2n) cross section (MT=16 → 24 in the new evaluation).
- Testing/benchmarking: (M. Herman, LANL) and thick-target angular neutron yields (Y. Danon, RPI) on the following slides

Comparison to previous ENDF/B Integrated cross sections: Well consistent, except inelastic, which is a bit below data, but there's no previous evaluations for that reaction

Testing/benchmarks Pencil-beam study: K. Parsons/LANL
Testing/benchmarks Lab spectra: Theoretical model expectation (G. Hale/LANL)
Lab elastic diff. scattering cross section excitation function (b/sr) at 26° as a function of E, the incident lab neutron energy (MeV).
Outgoing neutron TOF spectrum at 26° vs. t= 2236/sqrt(E) in ns. Incident energy (top axis), the first two resonances give structures at about 2400 and 2800 ns.

Testing/benchmarks Lab spectra: Quasi-integral simulation in MCNP (Y. Danon/RPI)
There are some differences when compared to VIII.0
Outgoing neutron TOF spectrum at 26° vs. t= 2236/sqrt(E) in ns. Incident energy (top axis), the first two resonances give structures at about 2400 and 2800 ns.

Testing/benchmarks Pulsed Be spheres
MCNP simulations (D. Neudecker/LANL) − Due to change (n,2n) & (n,n') evident near elastic peak − (n,2n) should probably be (has not been) reduced by (n,n')

Perturbative criticality study
M. Herman & W. Haeck (LANL)
New evaluation seems to perform worse. This has to be investigated and understood

Krusty testing J. Favorite (LANL/XCP-7)
"Krusty detailed models compared with the benchmark, ENDF/B-VII.1, and ENDF/B-VIII.0. We nailed it with ENDF/B-VIII.0. The new cross sections are a little better than ENDF/B-VII.1 but not nearly as good as ENDF/B-VIII.0."

n+16O evaluation

ENDF/B history
6.8, 7.1, 8.0

- ENDF/B-VI.8 (2001 April): LANL(Chadwick, Hale, Young), KAPL(Caro, Lubitz)
  - Below 3.4 MeV*: R-*function* + optical model (OPTIC code; Caro)
  - 3.4 < E_n < 6.25: LANL R-matrix (multichannel; EDA)
    - Data: n+^{16}O (total) [Johnson75, Larson80], ^{16}O(n,el) ang.[Lane60,…], ^{16}O(n,α_0) [inverse Walton et al.], ^{13}C(α,n), ^{13}C(α,el) excit. fn
  - E_n > 6.25
    - 6.25 → 20: subtraction of non-elastic (MT=3) from total
    - Inelastic (MT51, …, 57)
      - ^{16}O(n,xγ) Nelson, Chadwick, Michaudon & Young NSE99
  - MT800: Bair&Haas73 without renormalization
    - 6.2→20: factor of 1.5 "bring into rough agreement" (n,α_0) of Davis '63
  - MT801-803: inferred from (n,$\alpha\gamma$) [Nelson99]
- ENDF/B-VII.1 (2005 Dec.): VI.8+Page+Kawano+Young
  - MT=800: 32% reduction (n,α_0) 2.4→8.9 MeV
    - "assuming Harissopulos05 are definitive"; "Ha05 is 100% correct, BH73 100% wrong norm"
- ENDF/B-VIII.0 (2016 Dec.): VII.1+Hale+Kawano+MWP
  - Re-evaluation of Ha05 by Giorginis et al. (CIELO)
- JENDL-4.0 (2010)
  - ^{16}O(n,α_{tot}) < 6.5 MeV ~ ENDF/B-VII.0

ENDF/B comparisons ^{16}O(n,α_0)^{13}C [MT=800]
6.8, 7.1, 8.0

- Three regions
  - I. < 5.2 MeV
  - II. 5.2 → 6 MeV
  - III. > 6 MeV
- Trends
  - I. 7.1 < 6.8/8.0
  - II. ~Equivalent
  - III. 7.1 < 6.8 < 8.0

^{17}O Preliminary evaluation
Preliminary results

- Configuration: channels, R-matrix parameters
- Observed data in data deck
  - Channels: (*n,n₀*), (*n,n₂*), (α*,n₀*), (α*,n₁*), (α*,n*)
  - Types: total, integrated, differential, *polarization [A_y, P_n]*
- New data
  - Ciani *et al.* (2021) (α,*n₀*)
  - Brandenburg & Meisel (2021) (α,*n*)
  - Febbraro, DeBoer *et al.* (2020) (α,*n₀*), (α,*n₁*)

<u>17O system channel/pars</u>
- # channels: 45
  - $J^{\pi}=1/2^{\pm}$, ..., $11/2^{\pm}$
- # parameters
  - E_{λ}: 81 level energies
  - $\gamma_{\lambda,c}$: 322 reduced widths
- # Normalizations
  - n_M: 95 norm scales
  - ΔE_M: 4 shift factors

17O Preliminary evaluation Preliminary results: (?,n0) 13c(4he,n)16o dσ/dΩ E= 5.275 MeV
17O Preliminary evaluation Preliminary results: (?,n1) 13c(4he,n)16o1 dσ/dΩ E= 5.135 MeV
17O Preliminary evaluation Preliminary results: low energy

17O Preliminary evaluation scope Preliminary results

ENDF/B-VIII.0 16O(n,a_0)13C [MT=800] Comparison with New Evaluation "8.1"

ENDF/B-VIII.0 16O(n,a_0)13C [MT=800] Ratio of New Evaluation to ENDF/B-VIII.0

Preliminary new evaluation vs. OU(2021) & Bair & Haas(1973)

Outlook
- n+^{9}Be
  - the added inelastic data is well represented – why isn't it performing better?
  - Formatting? EDA_{f90}→ ENDF-6 correct?; ENDF-6 → ACE correct?
  - Is (n,2n) properly represented?
    - ^{9}Be(n,2n)^{8}Be* vs. ^{9}Be(n,2n)$\alpha\alpha$
  - ENDF/B-VIII.1 release push to Feb. 2024
    - re-assess available data
    - push to higher energies
    - update the evaluation & covariances
- n+^{16}O
  - Complete the evaluation to E_n ~ 9 MeV (maybe 10 MeV)
    - add missing data

        - Investigate normalization of the (n,n_{tot}) Cierjacks' '68 & '83 datasets
    - $^{13}C(\alpha,n_0)^{16}O$ is currently too high everywhere
        - Note that (n,n_{tot}) and (n,α_x) are tightly correlated by unitarity
    - Perform a complete normalization/covariance study

59Ni
14:40 - 15:10
Sean Kuvin

Study of 59Ni(n,p)59Co and 59Ni(n,a)56Fe at fast neutron energies

Outline
- Neutron induced charged particle measurements with LENZ at LANSCE
- Improved evaluation of outgoing charged particle spectra, built on ENDF/BVIII.0, for higher fidelity simulations of the LENZ experimental setuo
- Study of 59Ni(n,p)59Co and 59Ni(n,a)56Fe with a 59Ni target
    - Comparison to a surrogate ratio measurement
    - 59Ni is a significant background component to our measurement of 56Ni(n,p)
- Summary/outlook

LENZ: The Low Energy (n,z) experimental station
- Detect outgoing charged particles using double-sided silicon strip detectors in a compact setup close to the target sample
- WNR Facility at LANSCE: fast neutrons with a broad energy spectrum ~100s of keV to ~100s of MeV

Nuclear data needs for neutron-induced charged-particle reactions (n,z)
- Damage due to hydrogen and helium production in structural materials like Fe, Cr, Ni, etc.
    - Manuscript on 54Fe(n,z)/56Fe(n,z) to be submitted for publication
    - Measurements of 58Ni(n,z)/60Ni(n,z) with LENZ are under analysis (D. Votaw)
- Precision measurements of key reactions like 6Li(n,t)4He, 10B(n,a)7Li, 12C(n,a)9Be, 16O(n,a)13C, etc.

    - Reactions on carbon studied using a diamond detector as asn active carbon target, published in PRC
    - Differential cross section measurements on 16O(n,a)13C to be submitted for publication
- Informing the design of next-gen reactors (e.g. fast spectrum molten salt reactors where reaction slike 35Cl(n,p)35S can play a significant role as a neutron poison and produces 35S ($T_{1/2}$ ~ 75 days) that can complicate the path to certification for designs that incorporate chloride salts
    - Study of 35Cl(n,p)35S with LENZ published in PRC. Results presented at previous meetings
- Constraining the vp-process for nuclear astrophysics by studying (n,p) reaction on proton-rich unstable nuclei (radioactive targets). E.g. 56Ni(n,p)56Co (56Ni $T_{1/2}$ ~ 6days)
    - Data analysis underway for the study of 56Ni(n,p) with hotLENZ
- Radiochemistry diagnostics for quantifying performance of nuclear fuel burning
- LENZ: Low Energy (n,z) collaboration/experimental setup developed to pin down these types of reaction that are ubiquitous in nature. Measure double differential cross sections with respect to energy and angle with an emphasis on incident neutron energies between 200keV and 20 MeV
- Overall trend of the energy averaged cross section fairly weel reproduced by statistical calculations aside from the fluctuations.
- ENDF/B-VIII.0 slightly overestimates the cross section above 1.25 MeV and significantly underestimates it below 1.25 MeV
- Measurement of 56Co(n,p)56Fe in the latter days of the experiment provides clean signature of the 56Ni content at the beginning of the experiment and background characterization
- 59Ni(n,p) peak provides evidence of IPF produced nickel

Improved evaluations of (n,p) and (n,a)

- Include missing particle production spectrum, discrete states, angular information. ENDF/B-VIII.0 total cross sections unmodified (and partial cross sections when available)
- Modified evaluations for (n,p) and (n,a) were performed for 62 different isotopes by Hyeong-il Kim of KAERI and incorporated into the MCNP simulations
- H. I. Kim et al., Nucl. Instrum. Methods Phys. Res. A 964, 163699 (2020)
- Data libraries also generated for reactions on 56Ni, 57Ni, 56Co, 57Co, etc for which no previous ENDF/B-VIII.0 evaluation existed

Benchmarking (n,z) reactions between GEANT4 and MCNP

- Simulation of 63Cu(n,z) shows good agreement between MCNP and GEANT4 when ENDF/B-VIII.0 is used. However, the spectra is not realistic and does not reproduce the expected outgoing charged particle energies from experiment. Library includes total cross sections and energy-angle information (MF=6)

- However, when using the modified data library as an input, which includes partial cross sections to discrete states and angular distributions (MF=4), GEANT4 and MCNP are only in agreement after making modifications to the GEANT4 source code
- Development of the GEANT4 simulation is being led by P. Tsintari from CMU. A manuscript is expected to be submitted soon

59Ni(n,p)59Co and 59Ni(n,a)56Fe

- 59Ni is a long-lived ($T_{1/2}$ ~ 100,000 years) unstable isotope of nickel that is bookended between the stable A=58 and A=60 isotopes
- Can build up to a non-negligible portion of the total nickel content in reactors from neutron capture on 58Ni at thermal energies and from 60Ni(n,2n) at fast neutron energies in fusion reactors
- No prior experimental data on 59Ni(n,p) or 59Ni(n,a) at fast neutron energies above 20 keV, except for (n,xp) cross sections derived through a surrogate ratio method (SRM) above 10 MeV
- Measured with LENZ during the 2019 (~1 ug of 59Ni) and 2020 (~100ug 59Ni) run-cycles
- JEFF-3.3 includes the most recent evaluation of 59Ni from thermal to fast neutron energies
- New data allows for a sensitive test of calculations that use global input parameters and/or to benchmark indirect methods like SRM

Surrogate ratio measurement of 59Ni(n,xp)

- Prior to this work, the only available 59Ni(n,xp) cross section information at fast neutron energies was derived from a surrogate ratio method. Derived relative to 60Ni(n,xp)
- The scale and trend of their data was inconsistent with statistical calculations using default parameters and with ENDF, JEFF, and JENDL for which they conclude that new evaluations are necessary
- Modification to the proton optical potential used in the statistical calculations are proposed to reproduce the scale of their experimental data (scaling r_v by 1.25 relative to the default Koning-Delaroche potential).

New data on 59Ni(n,p) and 59Ni(n,a) at fast neutron energies

- Neutron fluence measured relative to 238/235U(n,f), 1H(n,el), and 6Li(n,t)
- Statistical Hauser-Feshbach calculations performed using the code CoH3 and with TALYS. Koning-Delaroche used for n+59Ni and p+59Co, and Avrigeanu et al. for a + 56Fe
- For (n,p) below 3 MeV, the experimental cross section is approximately 30% lower than the available evaluations and from the calculations using default parameters. In contrast to the adjustment of r_v by 1.25 by Pandey, we obtain better agreement with our data by more modest scaling adjustments of 0.9, 0.95 and 0.95 for the a_w, r_w, r_v proton OMP

Comparison between 59Ni(n,p)59Co and 59Co(p,n)59Ni

The prescribed adjustment by Pandey et al. (scaling the volume radius term by 1.25) to the default optical model parameters in TALYS also performs worse compared to the default parametesrs when reproducing the 59Co(p,n) data. It results in a factor 4-5 difference between our direct measurement data and the calculation for 59Ni(n,p_0) at ~2 MeV

In contrast, we obtain better agreement between the (p,n) data and our experimental (n,p) data with the more modest adjustments to the proton OMP.

Comparison with JEFF-3.3 and indirect measurement

- Going from the upper to lower bounds of the 1 sigma band from JEFF3.3 represents a range of nearly a factor of 5 and is inconsistent with the cross sections derived from the surrogate work.
- Our direct measurement is in fairly good agreement with the central value of JEFF-3.3 above En = 3 MeV but requires a slight adjustment below 3 MeV
- CoH3 calculation (blue), shoen with +/- 15% adjustments to the level density parameter, a.
- Raises questions about the reliability of that particular application of the SRM
- Direct measurements on radioactive isotopes should be made, when feasible.

Summary/Outlook

- New data 59Ni(n,p) via a direct measurement with a radioactive nickel target demonstrated the importance of making direct measurements, when feasible (manuscript written, to be submitted to PRC)
- Analysis of 56Ni(n,p) data is in progress
- In addition, recent measurements on 58Ni and 60 Ni (analysis led by D. Votaw) with LENZ will help provide a more complete evaluation of the nickel isotopes when combined with the radioisotope data.
- To have more predictive simulations of the LENZ experimental setup, we have made a modified evaluation that is built on VIII.0 but includes more accurate information on the population of discrete levels and outgoing angular distributions.
- In anticipation of some of the nuclear data needs for (n,z) reactions on unstable nuclei, we have bein planning the development of a solenoidal spectrometer for (n,z) studies at LANSCE that will have significantly improved sensitivity over a more “traditional approach” to charged particle detection.

A paper about this work has been published in Physical Review C after the 2022 CSEWG meeting: https://journals.aps.org/prc/abstract/10.1103/PhysRevC.105.044608

181Ta
15:10 - 15:40
Dr Mike Herman

ENDF/B-VIII.0 evaluation

- Originally ENDL-2009 evaluation created by running Talys-1.0 with default input parameters. In this context, ENDF/B-VIII.0 performs quite well although we will show a number of deficiencies.
- Some features:
    - spherical Koning-DeLaroche potential most likely with the CC,
    - Hauser-Feshbach with Moldauer width fluctuation and ang. distributions,
    - Gilbert-Cameron level densities,
    - two-gas exciton model for the pre-equilibrium emission,
    - isomeric cross sections (MF=10) not included.

Motivation:

- ENDF/B_VIII.0 description: "data file ...is part of a large collection of isotopic evaluations...not tested against experimental data ... only as good as the global quality of Talys. "
- Tantalum is used for casting of plutonium peats at LANL PF-4. k_eff for this casting is 2-3 times more sensitive to inelastic, elastic and capture on Ta than to the respective reactions on Pu239 (LA-UR-19-31175)
- Isomers abound in residual nuclei produced in interaction of fast neutrons with Ta so it is relevant to Radchem (LA-UR-21-23034)
- Evaluation of the resolved and unresolved region by ORNL/NNL has been recently submitted to NNDC.

Experimental data for fast neutrons (100 keV - 20 MeV)

- Exceptional wealth of exp. data for practically mono-isotopic (99.99%) Ta181
    - cross sections:
        - total
        - elastic
        - inelastic scattering
        - capture
        - (n,p)
        - (n,2n)
        - (n,α), (n,t), (n,3He), (n,nα),
    - Angular distributions
        - Elastic
        - Inelastic
    - n and γ DE an dDDX(+p&α)
    - Several isomeric cross sections

• Number of EXFOR datasets : 343
• Number of EXFOR quantities: 137
• EMPIRE makes 468 plots (!)
Extraordinarily well distributed measurements!

Concept of this evaluation

- Combine modeling of EMPIRE-3.2 with experimental data to produce a consistent picture of nuclear reactions considering "all" available differential and integral data.

Implications of the concept

- Evaluation totally defined by the code and its input (physics preserved)
- Selection of models given priority over adjustment of parameters (right physics)
- Ignoring experiments inconsistent with other experimental data or with general picture
- **Gradual use of experimental data in the model selection and parameter adjustment** ("don't fit OMP to capture")
- Limited model parameter adjustment (mostly manual)
- Global fitting of model parameters only at the very end (...if needed)

All the results presented below were obtained without global parameter fitting!

CC optical model - total x-sec

- Ta181 is a strongly deformed and requires Coupled-Channels (CC)
- The RIPL-3 (#610) regional CC potential extends up to 200 MeV but it needs adjustments from 50 keV up to 20 MeV
- Two reliable and consistent measurements of total by Poenitz et al, covering entirely this energy range were used to refine the potential
- Fitting performed with Kalman filter resulted in rather minor corrections

Scaling factors:
rv 0.98542
Vv 1.0184
av 1.0870
β2 1.0444
β4 0.93707
β6 0.49351

Five experiments that support the evaluated total compared with the CC calculations using updated optical potential.
LANL evaluation perfectly fits Rapp, Poenitz 81 & 83, Tsubone, Smith, and Carlson.

- Hannaske, and Byoun show the same shape as LANL evaluation and agree after ~3% and ~4.5% renormalization respectively. A 1.5% upscaling brings Foster into agreement.
- Finlay shape is slightly different but still within 2% of the new evaluation
- VIII.0 too high below 2 MeV and too low above 7 MeV

CC model - elastic x-sec & angular distributions

Elastic cross sections after adding the 1-st and the 2-nd inelastic.

Elastic angular distributions

The 1-st and the 2-nd inelastic angular distributions added.
At 4.5 MeV calculations underestimate Smith data, although the shape is quite good. Other experiments, however, are also lower...

This trend continues through the higher incident energies - Smith data are higher than the evaluation while other experiments agree.

CC model - inelastic x-sec
The 1-st inelastic (summed into elastic) does not belong to the ground state rotational band. The DWBA has been added to increase elastic angular distr. at higher energies (disregard numerical fluctuations)
VIII.0 cross sections are higher for this and other inelastics and agree better with experiments but.. it comes at a price of overshooting total by ~0.5 b.

2-nd inelastic
The first collective level at 136 keV above the g.s. Similarly to the first it is higher in VIII.0.

3-rd inelastic
Not collective in LANL calculations. In VIII.0 seems to be collective but the high- energy tale might also come from the PE contribution distributed over all discrete levels.

MSD/MSC - neutron spectra, inelastic & (n,xn)

- Quantum mechanical Multistep Direct (MSD) and Multistep Compound (MSC) were employed for neutron emission instead of the exciton model.
- MSD eliminates the need of adding large number of collective discrete levels to the continuum. Default calculations were pretty good but adjusting (manually) a single parameter brought additional improvement. MSD Io = 6.38 MeV
- Extensive experimental coverage of DDX from 5 to 20 MeV of incident energies at different angles was essential for building confidence in the calculations.

Angle integrated energy n-spectra
Three consistent data sets are well reproduced by the calculations.

Double-differential n-spectra
VIII.0 has a serious issue with all neutron spectra.
If Salnikov data were the only available it could be concluded that exciton model is enough to describe neutron spectra...
...which is obviously not true.

Even 30 deg at 20 MeV is well reproduced, but not 15!

This is a recurring problem and I wonder whether it is related to experimental difficulties related to beam neutrons scattered to the detectors?
MSD could also be blamed (compressional form-factor overshoots forward angle data).

Here, however, we have dramatic increase of the data below 5 MeV that is hard to understand.

Level densities - capture, inelastic, (n,2n) x-sec, neutron & gamma spectra, ...

- Gilbert-Cameron level densities were chosen over EGSM and microscopic Hartree- Fock-Bogoliubov because the former produce better capture cross sections between 1-3 MeV, and slightly better gamma spectra.
- The effect on the neutron spectra is mixed with GC working better at incident energies around 14 MeV while EGSM has an advantage at 20 MeV.

Inelastic cross sections
Ignoring data by Smith, Takahashi and Rosen as inconsistent with the overall picture.
Relatively good agreement with VIII.0.

(n,2n) cross sections
VIII.0 agrees a bit better with experimental data.
The difference could be eliminated with the parameter fitting. Newly developed level densities have a substantial impact on (n,2n) cross sections.

181Ta(n,2n)179gTa cross sections
Agreement has been improved by completing decay schemes.
Some data need to be disregarded.

Gamma spectrum
VIII.0 has better energy resolution below 0.1 MeV but present evaluation is closer to the data above 2 MeV

VIII.0 gives no gamma spectra above 1 MeV of incident neutrons.
The new evaluation covers the whole energy range up to 20 MeV.

Exciton model - charged particle emission
Exciton model is the only option in EMPIRE for charge- exchange reactions and cluster emission in the pre- equilibrium (PE) domain. With neutrons treated within MSD/ MSC there is more freedom to adjust PE yield.
(n,p) and (n,α) reactions required reduction of the mean-free-path multiplier from the default 1.5 down to 0.8.
MFP = 0.8
(n,p) evaluation was guided by Filatenkov's and by Semkova's data.

(n,α) reaction
VIII.0 was probably misguided by the old Mukherjee experiment.

Isomeric data confirm total (n,a) cross sections
Decay schemes completed to avoid default transitions to the g.s.

Modeling summary

- Coupled-Channels with adjusted dispersive Optical Model potential
- Multistep Direct (MSD) model for pre-equilibrium neutron emission.
- Heidelberg formulation of the Multistep Compound (MSC) model for pre-equilibrium neutron and γ-emission.
- Exciton model for pre-equilibrium proton emission.
- Exciton model with Iwamoto-Harada extension for pre-equilibrium cluster emission.
- Gilbert-Cameron model for level densities.
- Hauser-Feshbach with Moldauer width correction and BB angular distributions for compound nucleus decay.

Merge with the new RR/URR

- The two independent evaluations in RR/URR (D. Barry, J. Brown, M. Pigni, A. Lewis) and the present fast neutron-range evaluation show surprisingly good agreement at the 100 keV matching point
- We are working on solving a couple of mismatches inside URR
    - fast neutron capture lowered down to match the new resonance evaluation below 100 keV
    - work on increasing inelastic scattering in the URR region to match fast-neutron cross sections
- Current ENDF-6 does not allow for effective use of competitive width. Meantime...

We work on both evaluations to make them fully compatible in the whole URR

Validation

- FAUST/CRATER estimates

Promising trend indicated by the CRATER...
Much higher sensitivity with TEX

Conclusions

- Reliable fast-neutron evaluation can be entirely encapsulated in the reaction model and related input
- Ta181 is a particularly relevant case due to extraordinary coverage of various observables by differential experiments that offer much help and relatively little headache.
- Difference from the similar ENDF/B-VIII evaluation
  • more advanced modeling (CC OMP, MSD, MSC, decay schemes) • more careful selection of models and parameters
  • new experimental data
  • isomers
- Overall improved agreement with differential data and hints of better performance in integral testing

Updates to the n+63,65Cu Angular Distributions
15:40 - 16:10
Jordan McDonnell
Marco Pigni

INTRODUCTION

- This work updates neutron reactions on 63,65Cu
- Motivation: To correct deficiencies in benchmark performance since critical assembly configurations use Cu as reflector
- Adjusts the angular distribution data to improve benchmark performance
- Validation against copper-sensitive ICSBEP benchmarks is ongoing

SHIELDING BENCHMARKS

- The ENDF/B-VIII.0 evaluation was found to perform poorly in the Rez shielding benchmark above 4 MeV.
- INDEN has resolved this by adopting JENDL data above 4 MeV (R. Capote, private communication)

ANGULAR DISTRIBUTIONS

- This work endeavors to clarify the role of the copper angular distributions for the performance of the copper-reflected benchmarks.
- The work of Shaw et al suggested reverting the 65Cu File 4 to that of ENDF/B-VII.1.
- Transitioning smoothly between RRR and high energy treatments appears to be the path forward.

Benchmark Performance – Preliminary
Performance of copper-sensitive ICSBEP benchmarks
The 63Cu drives the reactivity high if mubar is too low. The VIII.0 angular distribution for 63Cu is the better starting point

Conclusions

- As expected, the performance of the benchmark suite is very sensitive to changes in the angular distribution data
- The quasi-differential measurements performed by Blain eta al. at RPI provide a valuable constraint. Furthermore, VIII.0 disagrees with their measurements consistently at 300 keV (the transition between RRR and high energy)

- The next step is to conservatively adjust the Legendre coefficients near 300 keV, validating performance against both critical benchmarks and the RPI quasi-differential measurements.

Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Nuclear Science and Technology Department
Building 817
P.O. Box 5000
Upton, NY 11973-5000

www.bnl.gov