AMPX Developments in FY2023

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NCSP Technical Program Review, February 20 – 22, 2024

OVERVIEW

AMPX development in FY2023 focused on preparing for the release and testing of ENDF/B-VIII.1.

- Updates for Thermal Scattering Law in ENDF/B-VIII.1
- Resolution of a SCALE Issue with Thermal Kernels
- Photonuclear Physics Support

TSL FILES: MIXED ELASTIC SCATTERING

In order to process TSL files with the new mixed-elastic scattering format, AMPX and SCALE need development effort.

- Processing in AMPX is under development and subsequent code review.
- Inclusion in SCALE has required discussion of how to do so – strategy will involve a new (internal to SCALE) MT number, propagating the change into the transport codes.

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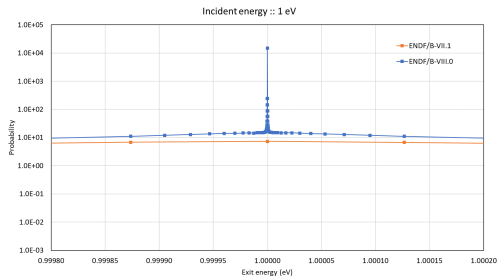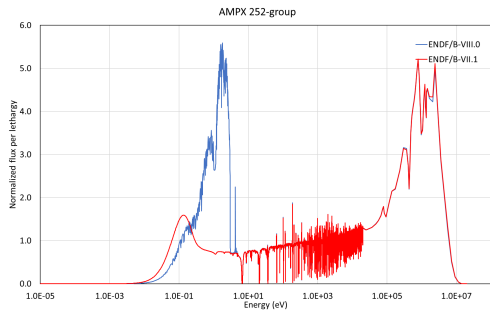## TSL FILES: SCALE CE LIBRARY FORMAT

The file sizes for the HDF5 format of the SCALE CE libraries:

- ENDF/B-VIII.0: 28 GB
- ENDF/B-VIII.1: 97 GB

Main contributor: The many Bragg edges in TSL files, which are represented in the SCALE CE library format in lab frame, double differential form.

Proposal within SCALE team: New CE library format that stores Bragg edges as a simple table, then samples "on-the-fly" during transport.

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THERMAL KERNELS WITH SHARP PEAKS – ENDF/B-VIII.0

AMPX 252-group

Incident energy :: 1 eV

- Using the ENDF/B-VIII.0 library to calculate self-shielding factors for a uranium pincell encountered unexpected PW fluxes.
- A long investigation traced this to the CENTRM handling of interpolation when encountering the sharp peaks in the h_in_h2o thermal kernel! This has been resolved by using an interpolation algorithm similar to corresponding points in CENTRM.

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AMPX PHOTONUCLEAR SUBLIBRARY SUPPORT

- Recent AMPX development enables the processing of the photonuclear sublibrary
  - Kalbach-Mann formalism for incident photons
  - Two-body physics for incident photons
  - Continuous energy and multigroup formats
- Coordinated development with the SCALE team in incorporating the physics updates into the Shift transport code
- The current SCALE 7.0.0 beta includes the photonuclear processing capabilities, the ENDF/B-VII.1 CE library, and a multigroup library with 31 neutron groups and 23 photon groups

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OTHER AMPX DEVELOPMENT HIGHLIGHTS

- Enhance PUFF processing of lumped reactions into covariances usable by SCALE

- Enhance performance of refined angular gridding (especially relevant for cryogenic moderators)

- Exclusive support for modernized (C++) POLIDENT code (point data and resonance reconstruction)

- Multigroup libraries with a 10 eV thermal cutoff, for both ENDF/B-VII.1 and ENDF/B-VIII.0, were updated with new homogenous f-factors to incorporate the effects of the fix to the CENTRM interpolation routines.

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CONCLUSIONS

- Updates for Thermal Scattering Law in ENDF/B-VIII.1
- Resolution of a SCALE Issue with Thermal Kernels
- Photonuclear Physics Support

AMPX available at
`https://code.ornl.gov/scale/code/scale-public`

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SPARE SLIDES

SPARE SLIDES FOLLOW

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GENERAL ENDF ISSUES ENCOUNTERED

Negative cross sections at 0 K:

- ^{54,57}Fe, ^{60}Ni, ^{141}Pr (each in MT=2)
- ^{65}Cu, MT=3
    - Corrected during the Hackathon, after Beta 2

Missing 1D data for: ^{14}N, MT=28,32

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GENERAL ENDF ISSUES ENCOUNTERED

Resonances with total widths greater than sum of partial widths ($\Gamma > \sum \Gamma_c$):

- Hg-203 (1500% relative change)
- Pm-144, Pm-145, Pm-146
- Tb-158, Tb-161
- V-49 (20,000% relative change)
- Yb-175

Note: AMPX (polident) uses the widths specified in the ENDF file, whereas NJOY resums. This is still in violation of the ENDF format.

Likely common ground: Files were produced by TALYS

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GENERAL ENDF ISSUES ENCOUNTERED

Incorrect NVER:

- Cr-50, Cr-52, Cr-53, Cr-54
- Fe-54. Fe-56 also has bad NLIB
- Se-78
- U-235 (also bad NLIB)
- Ta-181
- Te-122

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TSL FILES: WHICH FILE?

Case: I was running an ICSBEP ZEUS case which contains graphite.

Questions that arose:

- Which of the ENDF/B-VIII.1 graphite files most accurately represents the graphite used in that experiment? Should I simply use the crystalline graphite file? Choose a porosity…?
- Do I have enough information (i.e., from the ICSBEP Handbook) to determine which file most accurately represents the real material?
- Within SCALE, what can we do in the Standard Composition Library to continue making "correct" material specification easy for users?

TSL FILES: MANY TEMPERATURES…

Some of the TSL files have many temperature points (90).

Is this necessary?

Some of the temperature differences are under 5 K. Note that SCALE codes do not expect a granularity smaller than 5 K for the sake of Doppler broadening.

For the SCALE CE library: We will offer a subset of the temperatures specified in such files.

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AMPX PHOTONUCLEAR SUBLIBRARY SUPPORT

In processing the latest ENDF/B-VIII.1 Beta release:

- AMPX failed to process the Beta 1 ^{12}C file
  - Remedied by reverting to ENDF/B-VIII.0 ^{12}C
- AMPX failed to process ^{9}Be
  - Suspected in handling of MT=102 – needs further investigation
- AMPX did not find exit photon data for:
  - ^{44,48}Ca, ^{50,53,54}Cr, ^{19}F, ^{2}H, ^{3}He, ^{6,7}Li ^{180,182,183,186}W
- AMPX did not find 1D data for several reactions for:
  - ^{89}Y – MT=73
  - ^{169}Tm – MT=606,617, 632, 816, 830