OAK RIDGE National Laboratory

AMPX Status 2023

AMPX Team

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DISCUSSION OF AMPX and ENDF/B-VIII.1

- General ENDF issues encountered
- Issues particular to thermal scattering library
- AMPX Development Highlights
- Status of AMPX Photonuclear Sublibrary Support

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

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.

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.

Note: More than a change in CE data format, this imposes a change in the philosophy for SCALE transport codes. Up to now, the philosophy has been to represent reaction data as uniformly as possible (all lab frame, double differential, without needing special treatment for specific reactions)

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)
- Development of photonuclear sublibrary SCALE multigroup format

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
- 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

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

CONCLUSIONS

- AMPX processing has identified ENDF issues to correct for some files
- Several thermal scattering library files have presented a processing challenge, driving changes to the SCALE CE library format (for both processing and transport)
- AMPX's photonuclear sublibrary processing, for both SCALE CE and MG library formats, receives ongoing development

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

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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

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

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…

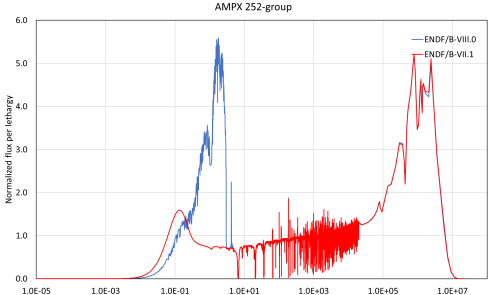
Some of the TSL files have many temperature points (90).

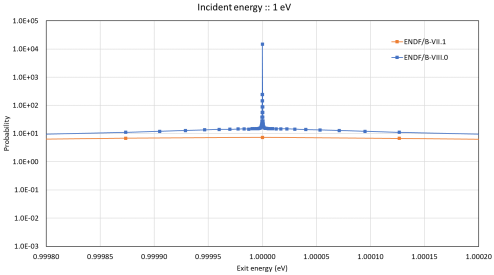
Is this necessary?

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.

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





- 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.