OAK RIDGE National Laboratory

AMPX Developments

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PUFF/COGNAC Improvements

- If it is a minor roundoff problem, we bump the values back into the valid range, and report it (as in SCALE 6.2)
- 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

SCALE 6.3 Data (cont.)

- 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.

 SCALE-6.3 is at RSICC! Deployed to our internal clusters, should be available for request to external folks soon™

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

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.

GNDS access layers in AMPX (cont.)

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.

GNDS access layers in AMPX (cont.)

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.

C++ classes support reading and writing.

We are in the process of updating to the upcoming GNDS-2.0.

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.

Future Plans

- Continue integration of AMPX and SAMMY components, focus on modern design and de-duplication, efficient storage
- Migrate AMPX R-Matrix calculation to take advantage of new SCALE/AMPX/SAMMY linear algebra interface
- Modernize PURM to improve run-time performance (perhaps use SLBW + Leal-Hwang doppler broadening)
- GNDS 1.9 -> 1.10 after 1.10 is finalized

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