OAK RIDGE National Laboratory

AMPX Status Report and ENDF/B-VIII.0 Data Testing

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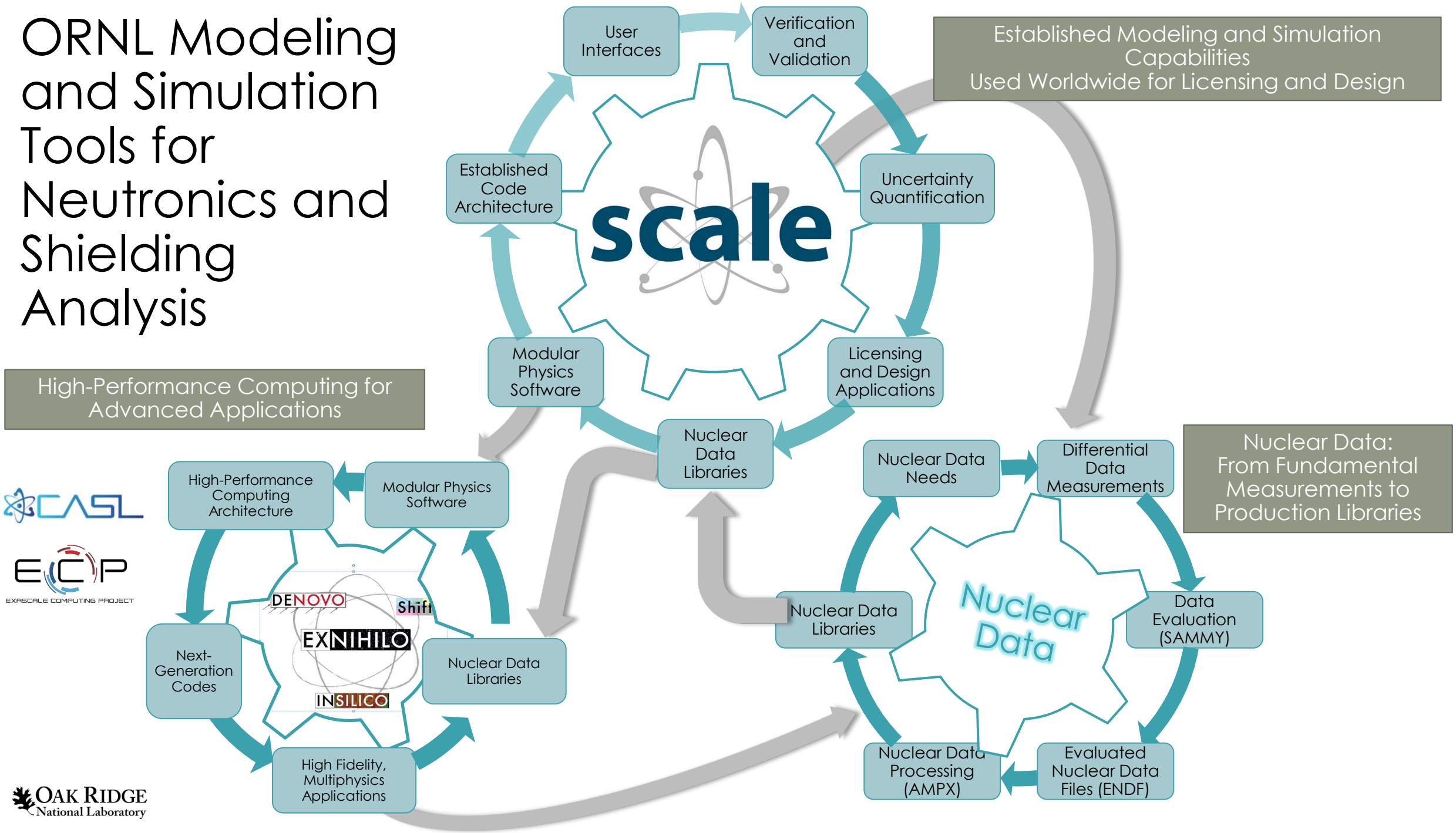
Overview

- Processing ENDF/B-VIII.0
- AMPX and GNDS
- Future plans to share code with SAMMY

ORNL Modeling and Simulation Tools for Neutronics and Shielding Analysis



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Processing of ENDF-B/VIII.0 library

- In order to process ENDF-B/VIII.0 an AMPX patch is needed.
  It will be available in the next SCALE beta.
  For previous versions the patch is available via email.
- In order to use the new moderator data in SCALE, a new Standard Composition Library is needed. It will be available in the next SCALE beta.
- Experimental libraries discussed in this talk will be available in one of the next SCALE beta releases.

Thermal moderators

In SCALE each moderator is bound with a suitable fast reaction and a unique ID. For example:

Thermal	Fast	Scale ID
Zr in ZrH	^{90}Zr	1040090
	^{91}Zr	1040091
	…	…

Unfortunately there is no easy pattern to:

- Automatically assign the nuclides to use in the fast region
- To assign a SCALE ID number.

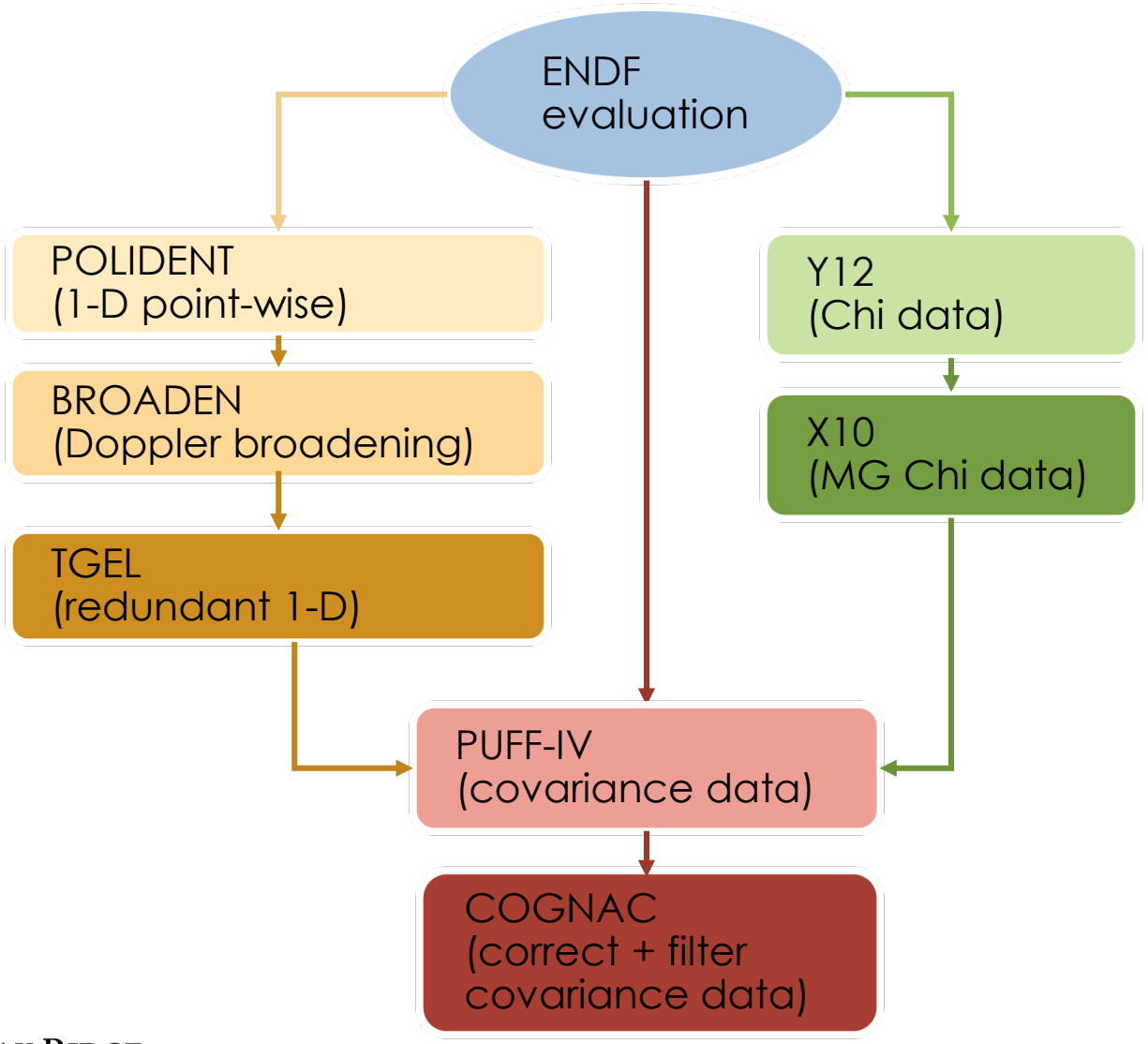
New ID numbers have been assigned and an appropriate configuration file has been written for use in generating inputs for AMPX.

ENDF/B-VIII.0 libraries

- CE library
- 252 neutron groups with homogenous f-factors.
- 302 neutron groups for use in fast systems
- 1597 neutron group library.
- Covariance library

Verification and Validation for these libraries is in progress.

Work-flow to generate the covariance library



- 1– D data are broadened to 293 K
- To collapse covariance data a Maxwellian-1/E-fission-1/E flux is used.
- A 56 neutron group library was generated.
- This library is expected to be available in the upcoming SCALE 6.3 beta release.

Corrections applied to SCALE covariance libraries

- All redundant covariance matrices are removed, i.e. if <1,2> and <2,1> are present, only <1,2> is retained. (Note: PUFF_IV adds these redundant matrices during processing).
- Cross section data without covariance information in the desired energy range are removed - i.e. threshold reactions outside the SCALE library energy range.
- Relative uncertainties larger than 100% are set to 100%
- Correlation values with absolute values larger than 1 are set to +1 or -1.
- If a higher energy group has uncertainty data and the lower energy groups do not (but have non-zero cross section data):
  - Diagonal elements of the covariance matrix are extended

SCALE ENDF/B-VIII.0 covariance library content

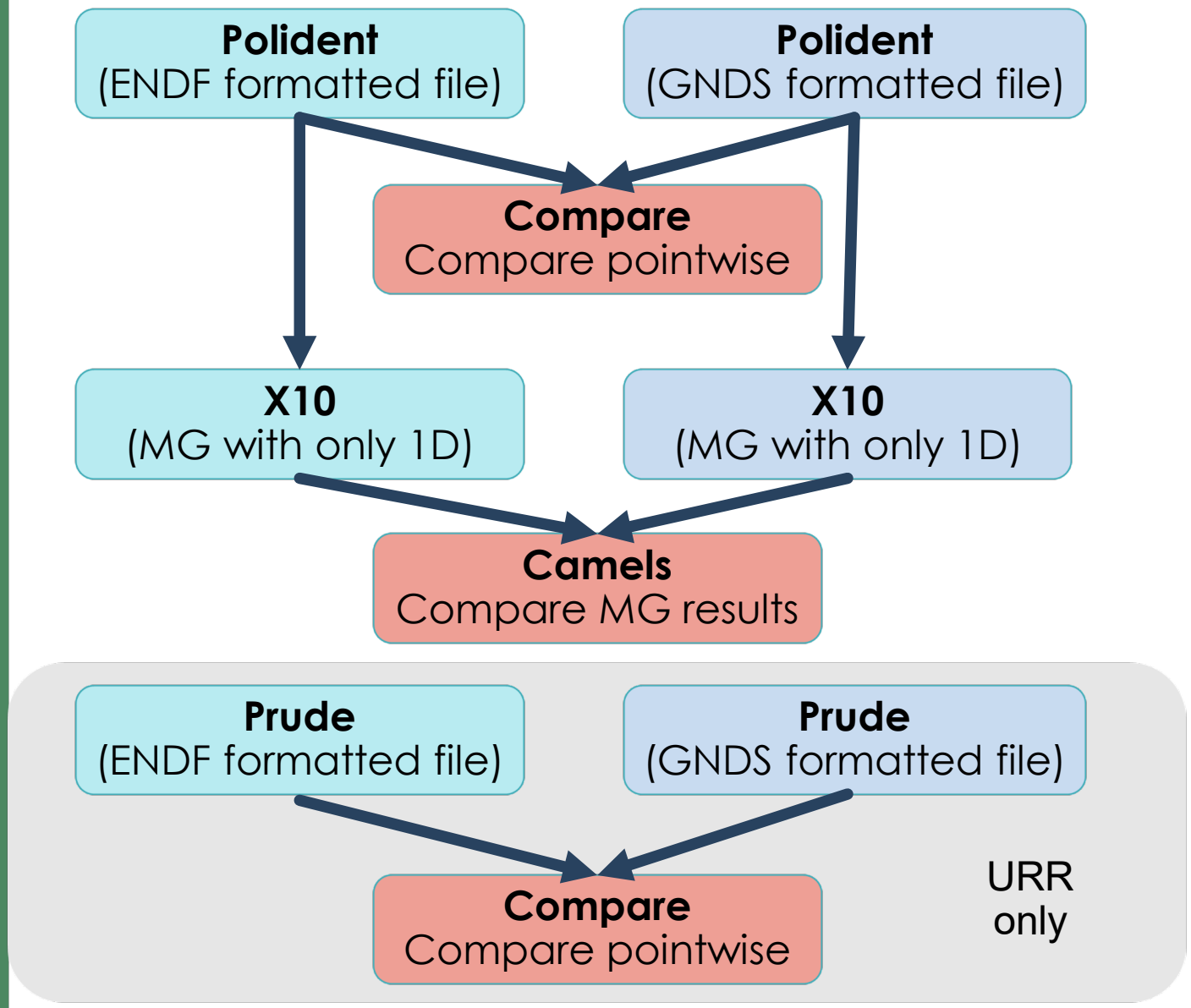
- All covariance information from ENDF/B-VIII.0
- Chi covariance data from JENDL-4.0:
  ^{241}Am, ^{242}Am, ^{243}Am, ^{237}Np, ^{231}Pa, ^{241}Pu, ^{232}Th, ^{233}U, ^{234}U, ^{236}U, ^{237}U
- SCALE-6.1 data (mainly Lo-Fi) retained for ~215 missing nuclides
- SCALE sensitivity tools currently only use the following reactions: 1, 2, 4, 16, 18, 102, 103, 104, 105, 106, 107, 452, 455, 456. Therefore these are the only reactions retained.

GNDS Access in AMPX

The "Onion" principle at work for GNDS access

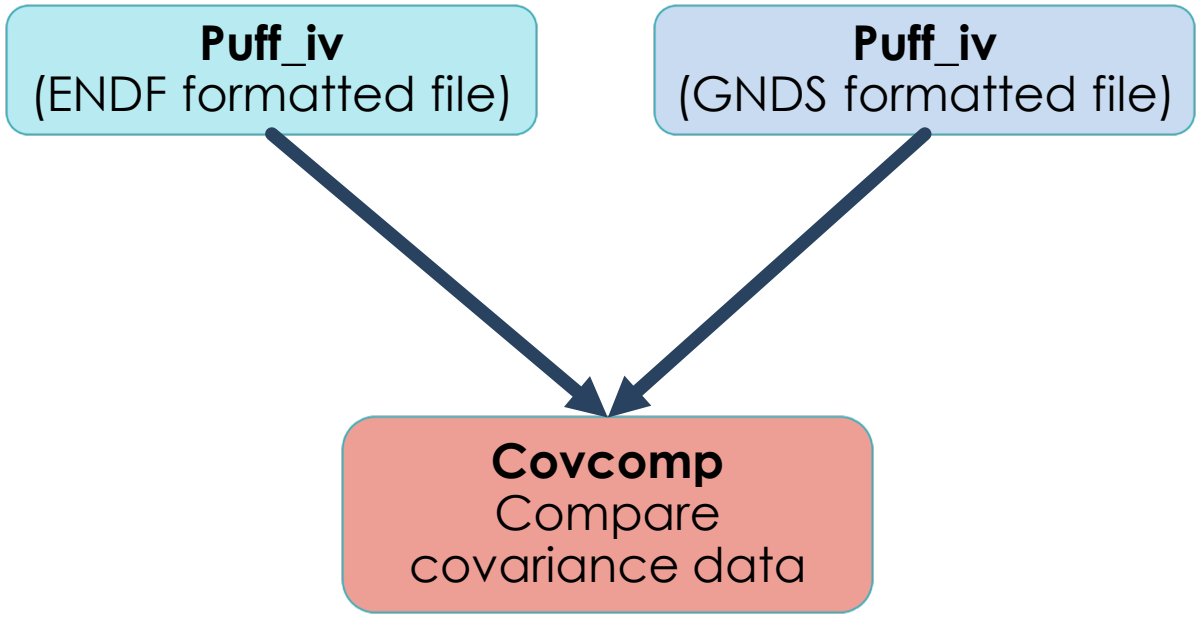
- File access:
  - API for file access, implementation for XML reading using QT XML parser
- General data containers:
  - Classes for all the general data containers used in GNDS
- GNDS structure:
  - Classes for GNDS structures (Cross section, Resonance data, etc.) needed by AMPX. These will be expanded as needed.
- AMPX and SAMMY in-memory structures:
  - Classes that fill AMPX in-memory structures from the classes in the GNDS layer and vice-versa.

1-D data including resonance reconstruction



- Generate a custom template for EXSITE that allows for generation of input files for all incident neutron evaluations
- ***Compare*** module makes a comparison of pointwise data on a union grid, but it does not signal missing reactions
- ***Camels*** module is used to catch missing reactions of grouped data
- ***Prude*** module processes unresolved resonance region (URR) data, whether for shielding only or also for point-wise cross section data

Test of covariance neutron data



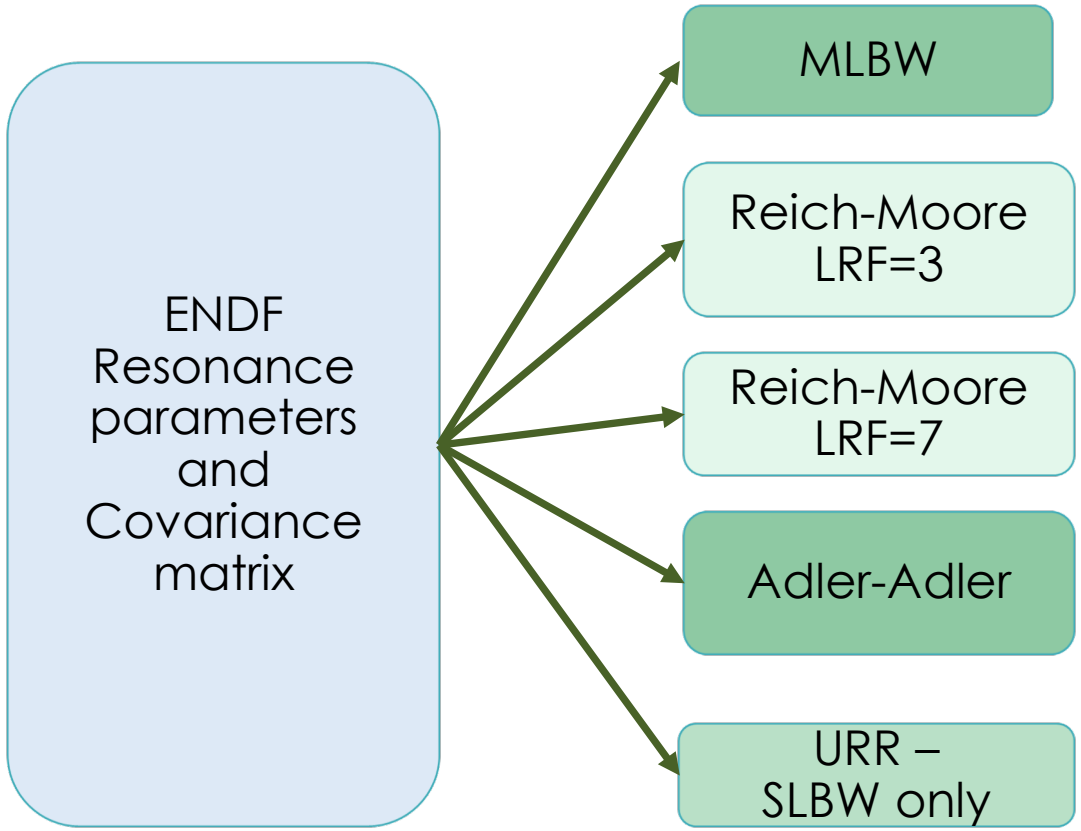
- Generate a custom template for EXSITE that allows the user to generate input files for all covariance data
- ***Puff_iv*** module can generate:
  - Cross section covariance data from pointwise data (File 31/33)
  - Cross section covariance data from resonance parameter (File 32)
  - Covariance data for CHI (File 35)
  - Each can be selected separately
- ***Covcomp*** module shows differences and missing covariance data

AMPX and SAMMY

- Since many of the same people are involved in AMPX and SAMMY development, we want to make code sharing easy.
- SAMMY and AMPX/SCALE will still be distributed as different codes, but contain the same code.
- Internally both codes are still in different source repositories, but shared code will only be contained in one of the repositories.

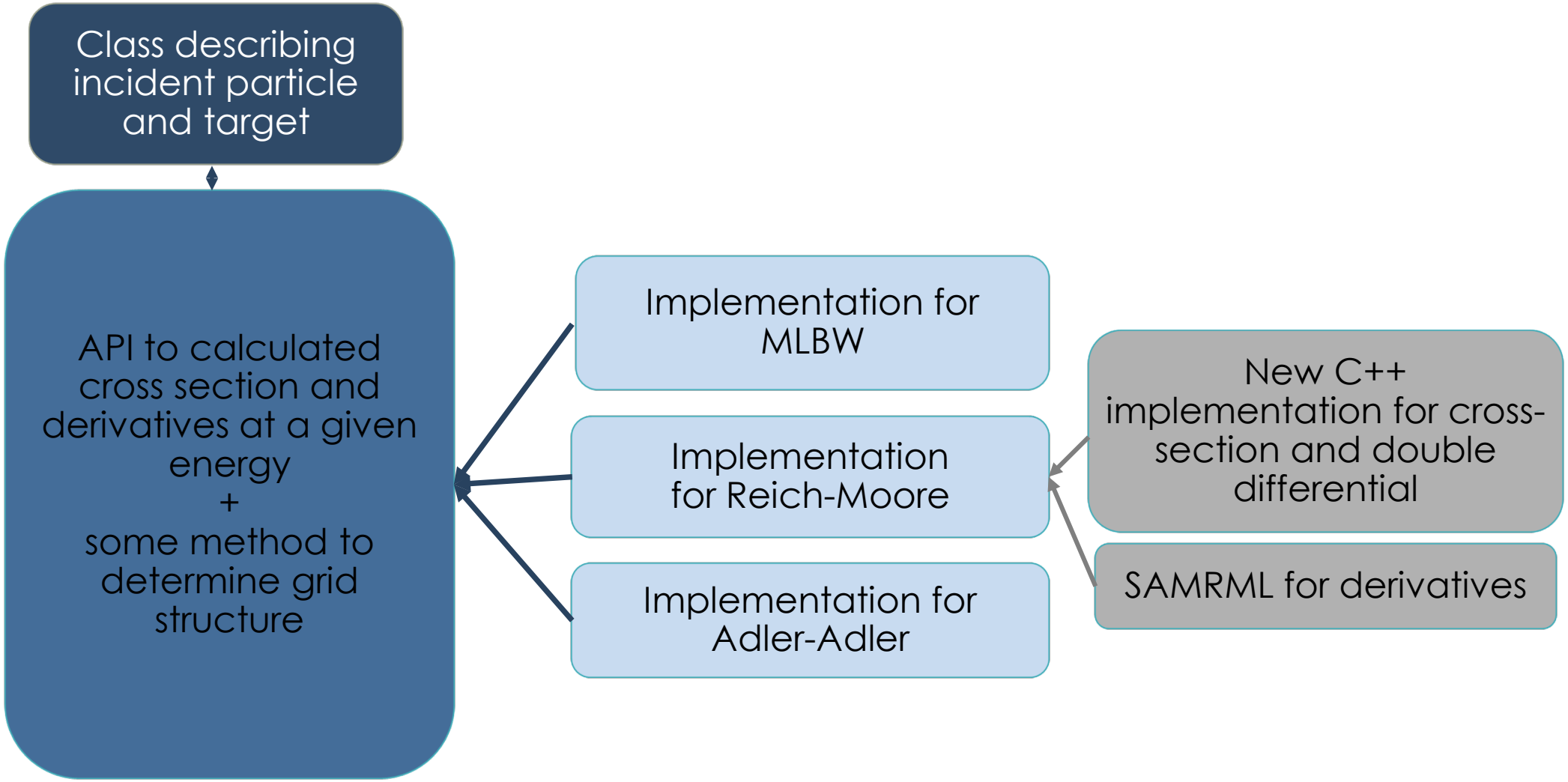
ENDF I/O

- AMPX already has a C++ ENDF I/O reader and (in many cases) writer
- API access to the ENDF data is independent of the ENDF file format (ENDF-6 or GNDS)
- We want to change SAMMY to use the AMPX ENDF API
- This will include extending the ENDF API as needed.



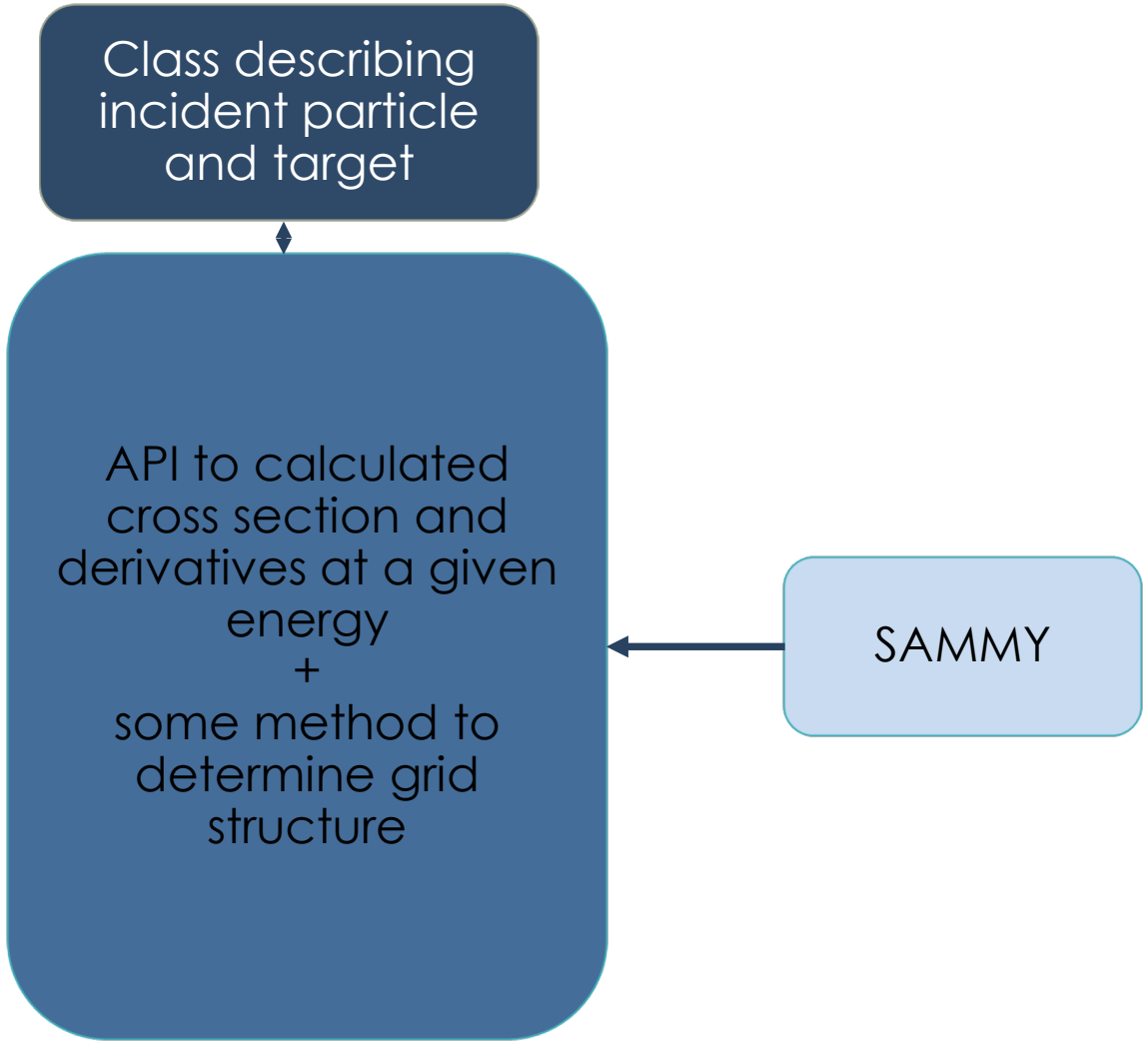
- SLBW and MLBW parameter are stored in the same class with a flag indicating which formalism to use
- Resonance parameters for Reich-Moore for LRF=3 are initially stored in a different class, but are converted to a LRF=7 class before calculation
- If derivatives are desired, all formalisms (except URR) are converted to LRF=7
- All resonance parameter classes can contain a covariance matrix. If converting to a different formalism, the covariance matrix is re-organized accordingly

Resonance processing as currently done in AMPX



Note: SAMRML is a simplified version of SAMMY where unneeded features are stripped.

Resonance processing as we want to do it



Advantage:

- One resonance processing code to maintain
- All new SAMMY features are immediately available in AMPX
- New ENDF format enhancements and algorithm changes are available in AMPX and SAMMY.

Summary

- New ENDF-B/VIII.0 CE and MG libraries have been produced and tested
- Work on implementing GNDS reading in AMPX progressed. Currently we are working on kinematic data.
- We plan more code sharing between AMPX and SAMMY