SAMMY Modernization Efforts

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Summary

- SAMMY releases

- Updates in the program flow

- Goals and Achievements in the Modernization Effort

- Updates for Broadening routines

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SAMMY and all dependencies are freely available

SAMMY 🌐
Project ID: 6231

https://code.ornl.gov/RNSD/SAMMY

SCALE-Public
Project ID: 11984

https://code.ornl.gov/scale/code/scale-public

- The build system has been updated

- A new version has been tagged (see next slide)

- The README has been updated, we are working on making installation even easier.

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SAMMY Version control

- We will tag Major and Minor versions as 8.1.1 etc.

- We will tag beta releases

- The specific version will be printed in the LPT file header

- Since users now have access to pre-beta releases, we will include the hash info (pre-beta untagged releases only).

- The information gets updated automatically after downloading and configuring.

```
*********************************************************
***                                                   ***
***      SAMMY Version 8.1.pre-b1 - 893ea39b          ***
***                                                   ***
*********************************************************

Name of input file:
```

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Updated SAMMY program flow

Because of the limited computer resources, SAMMY had a distributed and convoluted system to call the different modules.

Advantage:

- Each module (by way of global parameters) determines the next step in the calculation.

Disadvantage:

- The actual flow is very hard to follow as each module has to be examined as to where it directs the flow next.

- The same code appears multiple times:
  - For example: All Doppler broaden modules must point to the user desired resolution broadening function if and only if resolution broadening is wanted.

- Each module needs to have a lot of additional information regarding the user input.

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Consolidated the SAMMY program Flow

Consolidated blocks of related calls:

- One call to read input and parameter file

- One call to read data

- One call to handle:
  - 0K reconstruction (if desired)
  - Doppler broadening (if desired)
  - Multiple scattering (if desired)
  - Resolution broadening (if desired)

- Flow control handled in one Fortran module

Previously input and data were called multiply times, we attempted to minimize the calls, but still need to do more updates to avoid these multiple readings completely.

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Consolidated the SAMMY program Flow cont.

- Information like:
  - Resonance formalism, Doppler broadening formalism
  - Resolution function selection
  - Conversion to transmission
  - …

  Are now only needed in one place and not in any of the submodules, reducing the number of places global parameters need to be used.

- A better program flow allows for a better API through which external program (such as our FitApi program) can access SAMMY.
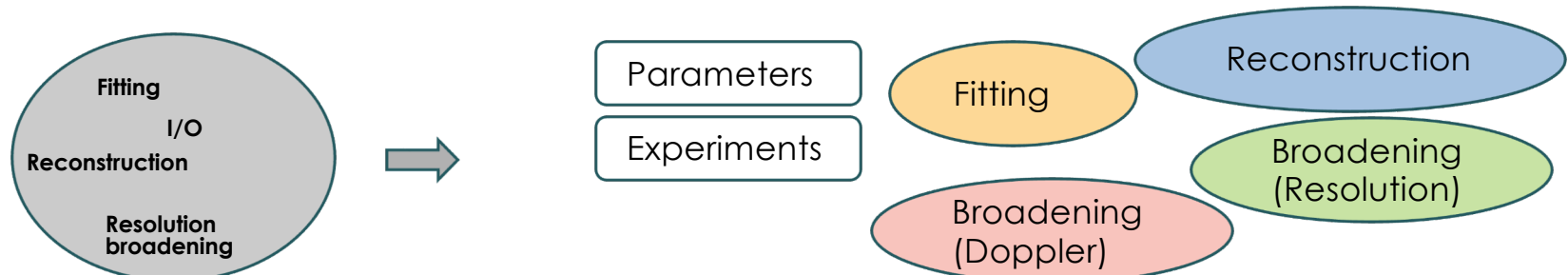
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SAMMY Modernization and Maintenance goals

We plan to modernize as follows:
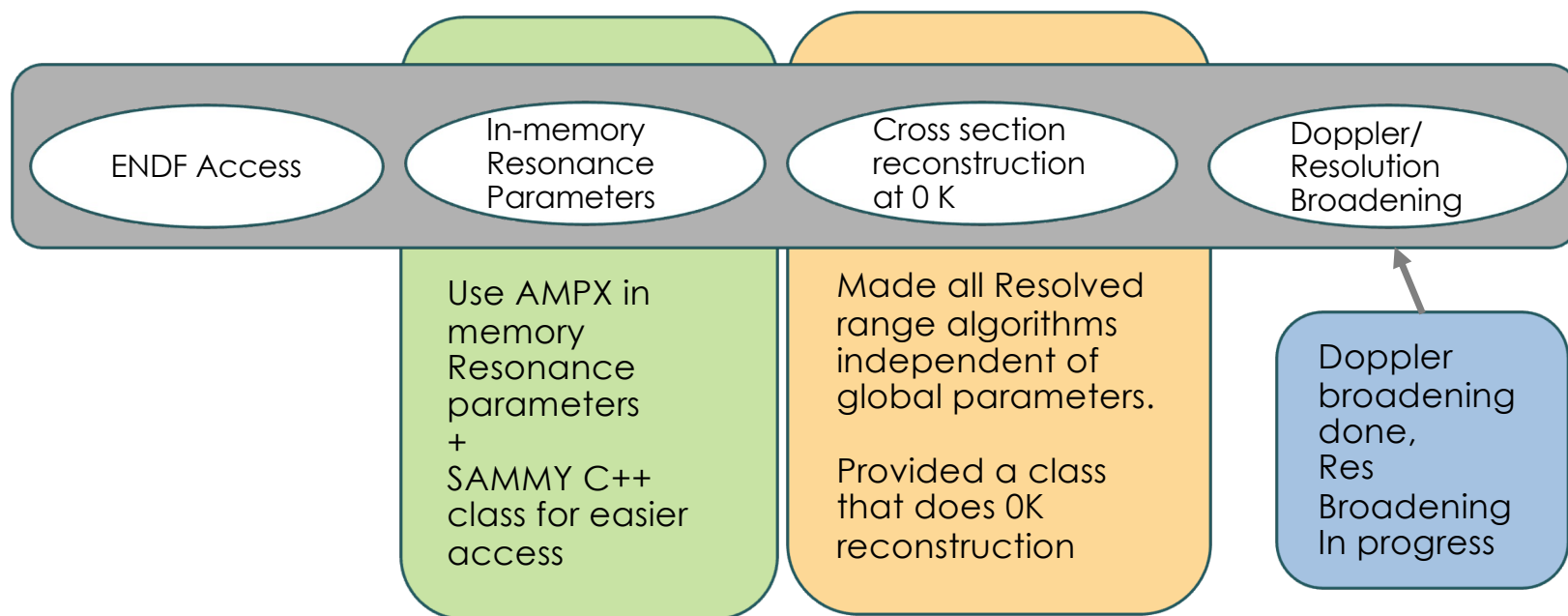
- Write code once and reuse
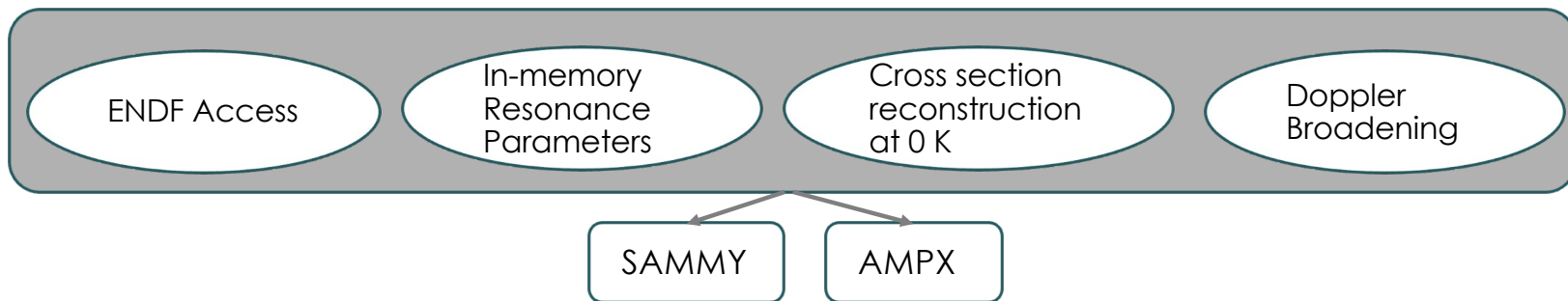
- Transform SAMMY into a modular code, with independent modules with clear interfaces.

- Add new features, which is now easier as only the desired module needs to be changed.

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SAMMY Modernization Accomplishments

ENDF Access

In-memory Resonance Parameters

Cross section reconstruction at 0 K

Doppler/ Resolution Broadening

Use AMPX in memory Resonance parameters + SAMMY C++ class for easier access

Made all Resolved range algorithms independent of global parameters.

Provided a class that does 0K reconstruction

Doppler broadening done, Res Broadening In progress

These modernizations will make adding new R-Matrix features easier as changes will be localized to the relevant part of the code as no global parameters are used. In addition, this will allow more parallelization of the code in the future.

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In memory C++ data classes

In order to manage the internal data in SAMMY, we are moving all data into C++ data classes. These classes just hold the data (with zero-suppression as needed (for example covariances)). User friendly access methods are provided in C++ and Fortran.

- Resonance parameters use the AMPX classes

- Covariances use the AMPX covariance class

- A SAMMY specific class holds cross section (per isotope) and derivatives as a function of energy

- SAMMY specific classes hold experimental data and covariance information

- A SAMMY specific class connects the internal parameters to their position in the covariance.

These classes provide convenient containers to pass around information without the need of global parameters.

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Doppler and Resolution Broadening

Parent class for all Broadening

Grid container (all energy info)
Derivative container
Internal temporary storage
Array of user parameters

Common function, mostly
concerning integration

- All Doppler and Resolution modules inherit from the parent class

- Implementation itself is unchanged and still in Fortran.

- While the user parameters are stored in the parent class, the interpretation is left to the module itself.

Having a common parent class, allows to select the Doppler Resolution method and Resolution broadening method(s) along with any user parameters at initial input reading.

Subsequent program flow does not need to have any information about the type of Doppler and Resolution broadening.

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Doppler and Resolution Broadening cont.

- The consolidation for the Broadening modules is finished for Doppler broadening and in progress for Resolution broadening.

- Unfortunately, the user parameters for the resolution broadening in the input file and in the covariance file are not collected in one block, but part of three difference sections: broadening, resolution broadening, additional parameters.

- This makes the consistent handling of these parameters extremely difficult, as the number and type of parameters of these sections depend on the broadening and resolution formalism.

The above mixing is an artifact of SAMMY developments predating the modernization effort. It was done to preserve backward compatibility with the input and covariance format.

Going forward, if introducing new features:

- We might break backward compatibility with the input and/or covariance format

- We will provide converters that convert to the new format.

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Global parameters

- SAMMY has a large number of global parameters

- Many of the global parameters have been eliminated in the modernization effort.

- Many remain, mainly related to the type of desired cross section and/or transmission and other experimental effects.

- Global parameters make it difficult to:
  - Use more than one normalization function
  - Fit the URR and RR together
  - Fit different experimental data together.
  - Use SAMMY via the external API (it needs to potentially be reset after every call)

- The next major effort will be to eliminate all global parameters.

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Conversion of user documentation to LaTex

- Documentation currently is given in a Word document

- This makes updating of the documentation difficult.

- A conversion to LaTex is in progress and the ASCII files are stored in the SAMMY repository.

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Switch to AMPX ENDF reading/writing routines

- It is planned to switch to the AMPX routines for access to the ENDF data. This will also give us access to the GNDS formatted file.

- We would also like to include information regarding the resolution broadening and normalization in a GNDS formatted file.

- This is currently in progress for the URR parameters.

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Conclusion

- SAMMY is available from https://code.ornl.gov/RNSD/SAMMY Versions will be tagged as needed.

- The program flow was improved to allow for easier external access to SAMMY routines.

- Modernization continued with the Doppler and Resolution broadening modules.

- Documentation updates are in progress

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