Oak Ridge National Laboratory

SAMMY Modernization Efforts in FY2018

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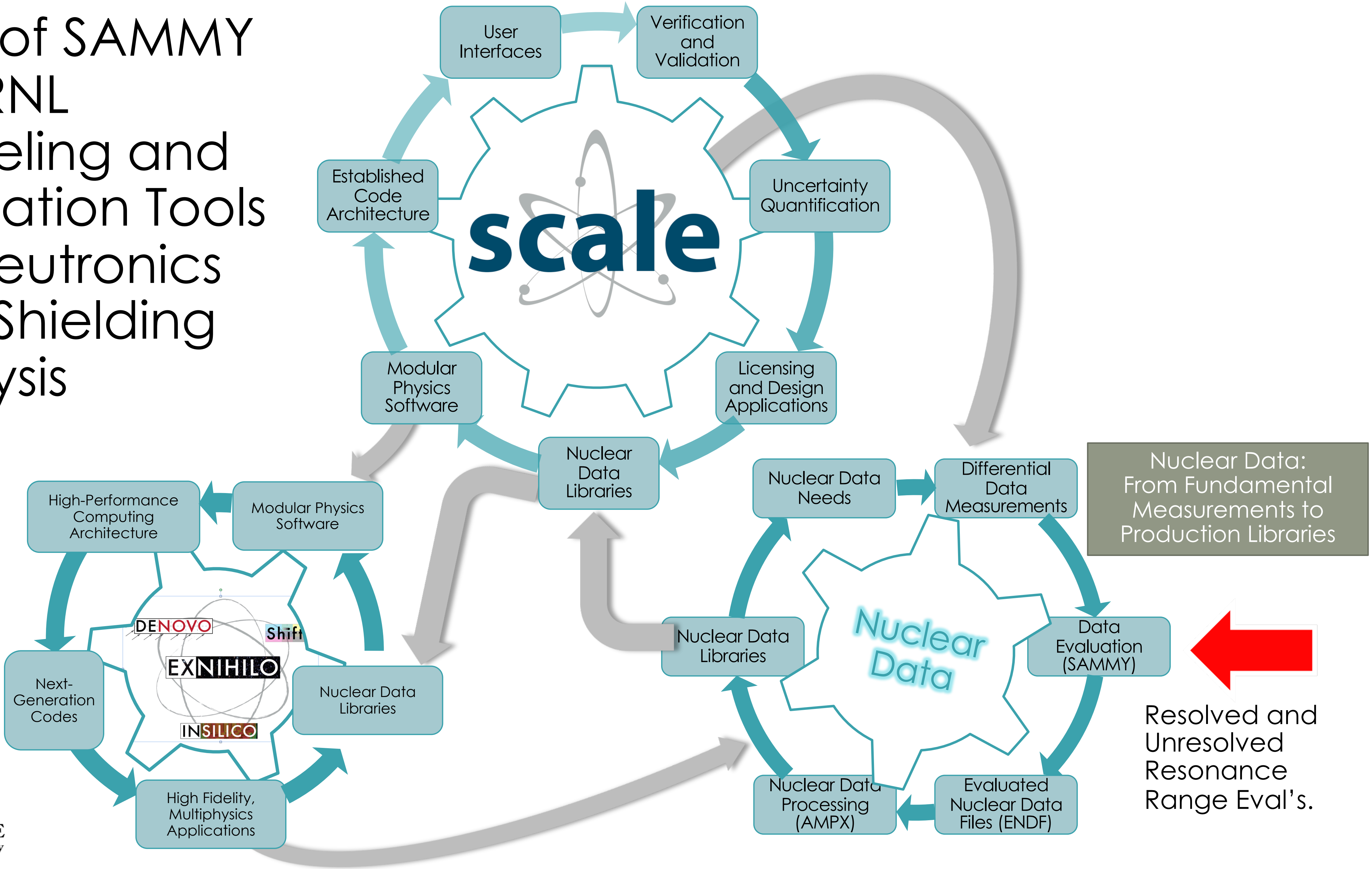
Role of SAMMY in ORNL Modeling and Simulation Tools for Neutronics and Shielding Analysis



Resolved and Unresolved Resonance Range Eval's.

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Outline

- Brief overview of SAMMY history and features
- SAMMY modernization strategy
  - API-based code-sharing with AMPX/SCALE
- SAMMY modernization accomplishments in FY2018
  - Modernized Coulomb functions
  - Inclusion of closed channels in the R-matrix
  - Transformation of formal to physical R-matrix parameters (a.k.a. Brune transform)
  - Replacing of Fortran COMMON blocks by modules
- SAMMY goals for FY2019
  - ENDF/GNDS AMPX API integration into SAMMY
  - New R-matrix resonance parameter fitting options
  - Open Source licensing for SAMMY 8.2 release
- SAMMY expansion roadmap

History of SAMMY

- Developed by Dr. Nancy Larson since 1970's
- Includes SAMMY + 25 auxiliary codes
  - (e.g., SAMRML shared by AMPX and NJOY)
- Architecture is a large Fortran (77) container array for memory management
- Includes 185 multi-step test cases + 10 tutorial examples
- Comprehensive documentation available at: http://info.ornl.gov/sites/publications/files/Pub13056.pdf
- Employed for resolved resonance evaluations in ENDF
  - Used for all ORNL nuclear data evaluations in Marco Pigni's talk
- SAMMY 8.1 distributed via RSICC https://rsicc.ornl.gov/

SAMMY capabilities

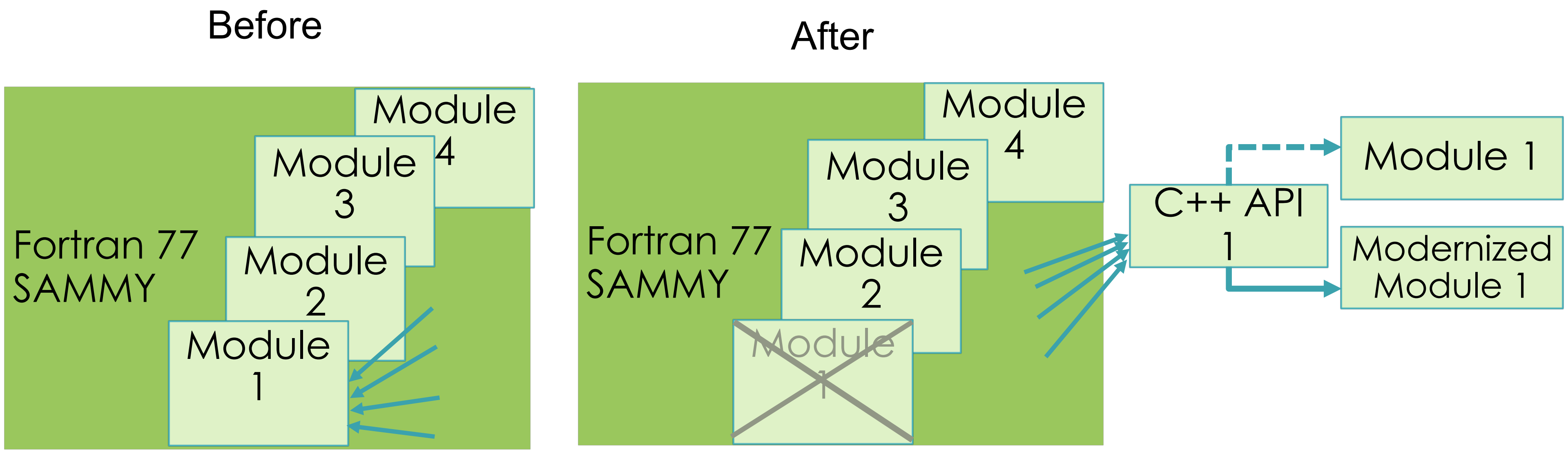
- Multilevel, multichannel R-matrix code
- Bayesian fitting of R-matrix resonance parameters (RPs)
  - Also known as generalized least squares
  - Yields covariance matrix of RPs
- Data reduction:
  - Experimental facility resolution functions: RPI, GELINA, nTOF, ORELA
  - Normalization, background
- Detector resolution functions: configurable for variety of detectors
- Doppler broadening: Solbrig's kernel, Leal-Hwang method
- Multiple scattering effects and other target effects
- Neutrons and charged projectiles: p,α
- Unresolved resonance range (FITACS by F. Froehner)

SAMMY modernization features introduced in 8.1:

- SAMINT: integral benchmark experiments inform research parameter evaluations (V. Sobes, L. Leal, G. Arbanas, https://info.ornl.gov/sites/publications/Files/Pub50343.pdf)
- SAMMY was integrated into SCALE software quality assurance (SQA) in AMPX footsteps
  - Automated cmake/ctest suite, revision control repository, FogBugz
  - Platforms supported: Linux/gfortran, Mac/gfortran, Windows/ifort
- New detector resolution functions were developed in collaboration with Rensselaer Polytechnic Institute (RPI)
- Updated physical constants, which are identical in SAMMY and SAMRML
- Implemented several other bug fixes and added 6 regression test cases

Modular modernization of SAMMY using APIs

Schematic diagram of SAMMY Fortran 77 legacy module modernization



Accomplishment 1: modernization of Coulomb functions

- **Background:** Coulomb functions are used in SAMMY to compute the R-matrix Shift and Penetrability functions needed to compute cross sections for charged-particle projectiles
- **Problem:** Shift functions are needed at negative energies for evaluations spanning channel thresholds but cannot be computed by SAMMY
- **Solution:** Coulomb functions will be modernized via the C++ API method outlined on the previous slide:
  - Leverage modern C++ Coulomb functions published by N. Michel 10.1016/j.cpc.2006.10.004
- **Issues:** 3 variants of Coulomb, Shift, and Penetrability functions are called in the legacy SAMMY depending on the values of input parameters; negotiated an Oak Ridge National Laboratory (ORNL) lab-wide license for use and distribution of Coulomb functions
- **Benefit:** Enables inclusion of channels below their thresholds (Acc. 2); enables conversion from R-matrix parameters to (and from) the Brune’s alternative R-matrix (Acc. 3), or the S-matrix poles, also known as Hwang “multipole” representations

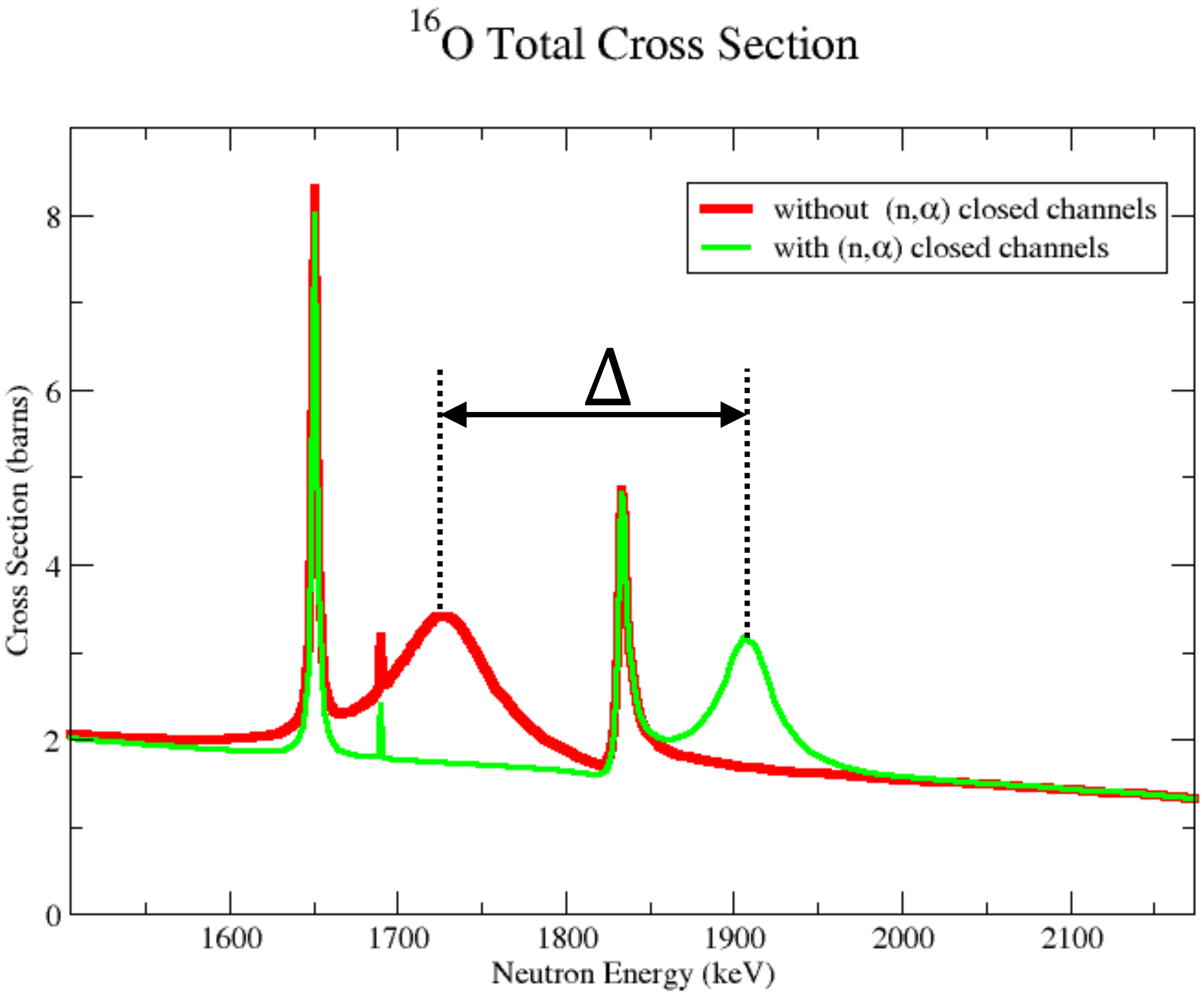
Acc. 1: modernization of Coulomb functions

- Code sharing of Coulomb functions with AMPX/SCALE
- N. Michel, "Precise Coulomb wave functions for a wide range of complex ℓ, η and z", Computer Physics Communications, Volume 176, Issue 3, 1 February 2007, Pages 232-249, http://doi.org/10.1016/j.cpc.2006.10.004.
- Several test cases re-baselined with more accurate solutions
- NEW test case added for Coulomb functions using high precision tabulated values
- Analytical simplifications for eta >> rho were retained to avoid numerical difficulties
- Analytical expressions for derivatives of the R-matrix shift function, penetrability, and the phase shift for charged particles have been implemented for the first time in SAMMY
  - Previously computed numerically for charged particles,
  - already computed analytically for neutrons

Acc. 2: Closed channel in SAMMY *R*-matrix

- **Background:** Historically SAMMY has been used for RRR nuclear data evaluations *below* threshold energy of the 1st channel. Consequently, including closed channels in the R-matrix was not needed.
- **Problem:** SAMMY is increasingly being used for RRR evaluations *above* the threshold energy 1st channel. R-matrix formalism requires this channel be included in R-matrix even below the threshold.
- **Solution:** Extend the dimensions of R-matrix (in channel indices $R_{cc'}$) to include closed channels below the channel threshold energy. Analytical expression for derivatives of cross sections w.r.t. R-matrix resonance parameters has been adjusted accordingly.
- **Benefit:** Enables evaluation of RRR above the the threshold energy of 1st reaction channels:

Acc. 2: Inclusion of closed channels in SAMMY

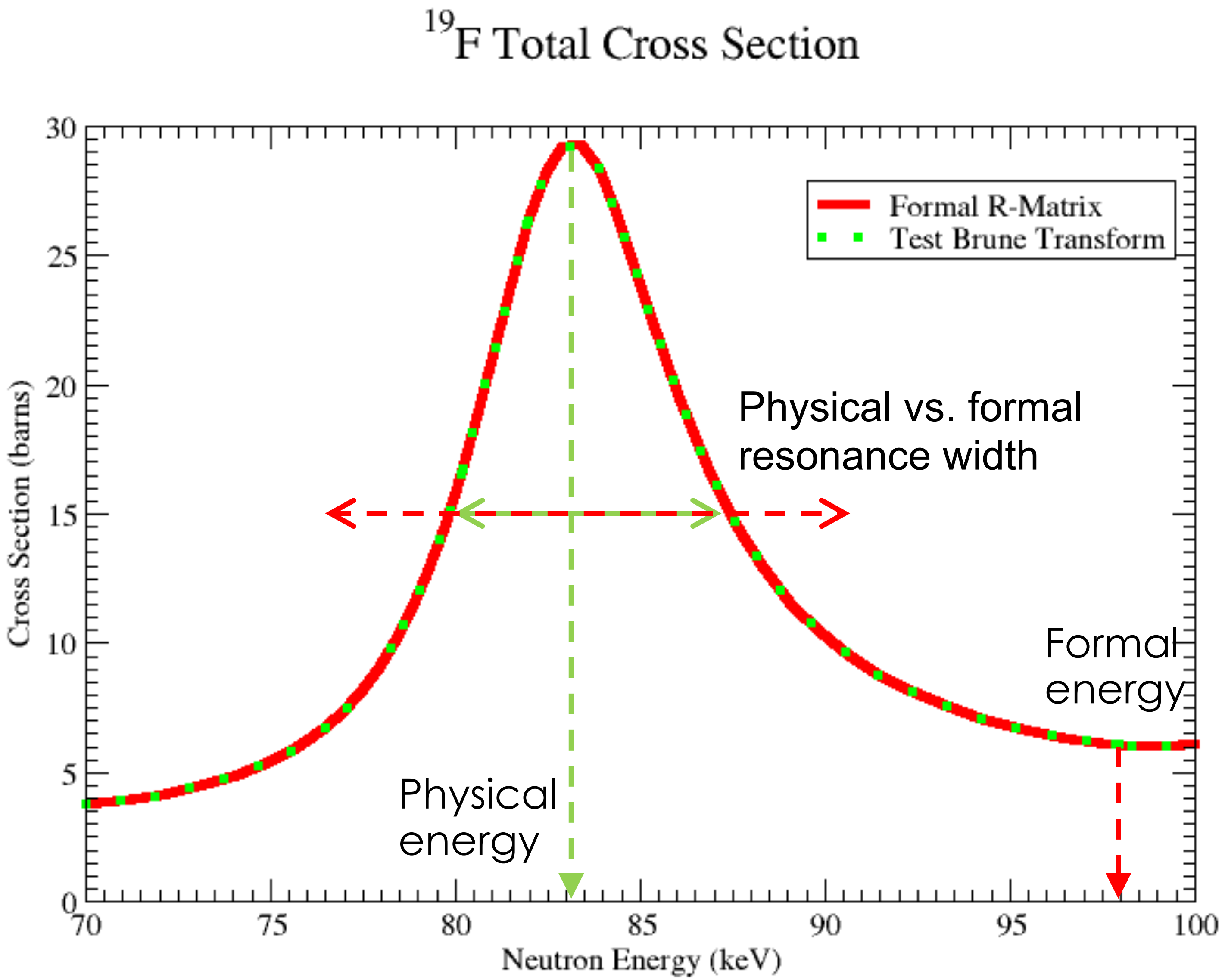


Δ: resonance energy shift due to (n,α) closed channel width (threshold energy of 2.355 MeV).

Acc. 3: Computation of "physical" R-matrix parameters

- **Background:** Resonance parameter compilations report resonance energy as the location of its peak and its width as the FWHM of that peak
- **Problem:** SAMMY 8.0 implementation employs <u>*formal*</u> R-matrix parameters, whose energy and width often do not correspond to the position and the FWHM of the peak. This makes correspondence between resonance parameters and peaks unintuitive.
- **Solution:** Implement conversion between <u>*formal*</u> and "<u>*physical*</u>" R-matrix parameters using a method derived by Carl Brune, Phys. Rev. C **66**, 044611 (2003).
- **Benefit:** Physical R-matrix parameters provide intuitive set of resonance parameters and enable straightforward comparison to legacy compilations of resonance parameters, e.g., Said Mughabghab, Atlas of Neutron Resonances, 6^{th} Edition (2018).

Acc. 3: Physical R-matrix resonance parameters in SAMMY



Acc. 4: Replacing COMMON blocks by F90 MODULES

- Few weeks of concentrated efforts by Wiarda, Holcomb, Arbanas, Chapman
- On the order of ~100 COMMON blocks in separate files
  - Each common block could have up to ~100 variables or arrays
  - Each subroutine INCLUDEs several of these files
- Replaced each COMMON block file by a corresponding F90 module
- In-house Perl Script to globally replace each INCLUDE by a USE module statement
- SAMMY test cases re-run after global replace for each file
  - Any failing tests would then be resolved
  - The last few particularly difficult ones were resolved by Doro
- All COMMON block replaced and all test cases passing

SAMMY long-term expansion roadmap

- **Background:** Nuclear theories, measured data, and optimization methods are becoming more sophisticated
- **Problem:** Although SAMMY is robust, its methods must advance
- **Solution:** Conceptual advances in evaluations methods are needed for cross section models and data optimization methods
- **Benefits:** Conceptual advances pave the way for advanced functionality

Simultaneous evaluations of thermal and resolved resonance region (RRR)

Bayesian optimization of defective models and incomplete data covariances (GLS and MC)

Parameterizing direct capture by a complex R-matrix channel radius; (cf. thermal complex scattering length)

Generalized Reich-Moore approximation and its Brune transform

SAMMY 8.2 anticipated features in 2019

1. Incorporate a C++ Coulomb function library CWFCOMPLEX into SAMMY/AMPX
2. Include closed channels in the SAMMY R-matrix (IAEA R-matrix collaboration)
3. Include closed channels in computation of analytical derivatives of cross sections inside SAMMY
4. Correct the bugs in the SAMMY I/O of ENDF files for charged particles by linking to the modern C++ ENDF I/O AMPX library
5. New R-matrix parameter fitting options
6. Update SAMMY documentation accordingly.
7. Release SAMMY under an open source license

Summary and outlook

- SAMMY is under the SCALE SQA framework
- Modernization proceeds via API framework
  - Coulomb functions
  - Inclusion of closed channels
- Code sharing with AMPX/SCALE (D. Wiarda, A. Holcomb)
  - guarantees consistency and is conducive to new data formats
- New evaluation concept developed for SAMMY long-term expansion
  - Simultaneous evaluation of thermal and resolved resonance ranges
  - New Neutron Capture formalisms for resonant and direct capture
  - Bayesian optimization framework for defective models
- Open source SAMMY release is in progress, as well as AMPX
- SAMMY 8.2 is expected later in 2019

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