

Modernization efforts for the *R*-Matrix code SAMMY*

Dorothea Wiarda¹, Goran Arbanas¹, Jesse M. Brown¹, Andrew M. Holcomb¹, and
Marco T. Pigni¹

¹Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The R-Matrix code SAMMY [1] is a widely used nuclear data evaluation code focused on the resolved range, which includes corrections for experimental effects. The code is still mostly written in Fortran 77, and uses a memory management system suitable for the time of its initial writing (1984). A modernization effort is under way to bring the code in-line with modern software development practices. A continuous-integration testing framework was added, automating the large existing set of test cases. It is run on every commit. The memory management was updated to current standard practices suitable for modern software analysis tools. The code can be obtained from <https://code.ornl.gov/RNSD/SAMMY>.

The resonance parameters and covariance information are now stored in C++ objects shared by SAMMY and AMPX [2], the processing code that generates nuclear data libraries for SCALE [3]. This allows for easier maintenance and access to the resonance parameters inside and outside of SAMMY. This feature is already used by accessing and changing parameters in memory in the Bayesian Monte Carlo Evaluation Framework for Cross Sections Nuclear Data and Integral Benchmark Experiments project [4].

Further plans include the switch to the ENDF reading and writing routines in AMPX, as these routines are more robust, easier to maintain, and support more features. Of note here is support for the new GNDS format [5]. Previously it wasn't easy to share the full covariance matrix for evaluations containing more than one isotope due to limitations on the ENDF format; this is now supported in GNDS. The data are currently available in a binary SAMMY format and can be exported to GNDS to make them more widely available and sharable.

The next step will be to use the same resonance processing code at 0K in AMPX and SAMMY as one of the available Reich-Moore R-Matrix formalism. The first step toward this goal is to isolate the reconstruction into a module that takes resonance parameters as its input and does not depend on SAMMY global parameters. This goal has been

*This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy (DOE). The US government retains and the publisher, by accepting the article for publication, acknowledges that the US government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for US government purposes. DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (<http://energy.gov/downloads/doe-public-access-plan>).

achieved and it should now be possible to more easily change the resonance formalism and add enhancements as the Phenomenological *R*-Matrix parameterization of direct, doorway, and compound nuclear reactions discussed elsewhere on this conference. This concerted modernization and enhancement effort provides multiple advantages to the nuclear data community. It will allow parameter optimization using enhanced formalisms, including experimental effects, that better match complex experimental data. Then those evaluated parameters can immediately be passed off to AMPX to be reconstructed with the exact same cross section model and be put into a data library for subsequent testing using SCALE and the Valid Benchmark suite [6] or other suitable benchmark suites.

Acknowledgments: This work was supported by the U.S. Department of Energy (DOE) Nuclear Criticality Safety Program, which is funded and managed by the National Nuclear Security Administration for DOE.

References

- [1] N.M. Larson, “*Updated Users’ Guide for SAMMY: Multilevel R-matrix Fits to Neutron Data Using Bayes’ Equations*”, ORNL/TM-9179/R8 (2008)
- [2] D. Wiarda, M. L. Williams, C. Celik, and M. E. Dunn, *AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications*, International Conference on Nuclear Criticality Safety (ICNC 2015).
- [3] W. A. Wieselquist, R. A. Lefebvre, and M. A. Jessee, Eds., *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.4, Oak Ridge National Laboratory, Oak Ridge, TN (2020).
- [4] G. Arbanas, J.M. Brown, A.M. Holcomb, and D. Wiarda, *Bayesian Monte Carlo Evaluation Framework for Cross Sections Nuclear Data and Integral Benchmark Experiments*, in the proceedings of the ANS Winter Meeting, NCSP Session (2020)
- [5] Specifications for the Generalised Nuclear Database Structure (GNDS) <https://www.oecd-nea.org/science/wpec/documents/7519-GNDS.pdf>, (accessed September 15, 2021).
- [6] W. J. Marshall and B. T. Rearden, *The SCALE Verified, Archived Library of Inputs and Data – VALID*, ANS NCSD 2013 - Criticality Safety in the Modern Era: Raising the Bar, Wilmington, NC, September 29 –October 3, 2013, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2013).