SAMMY Modernization

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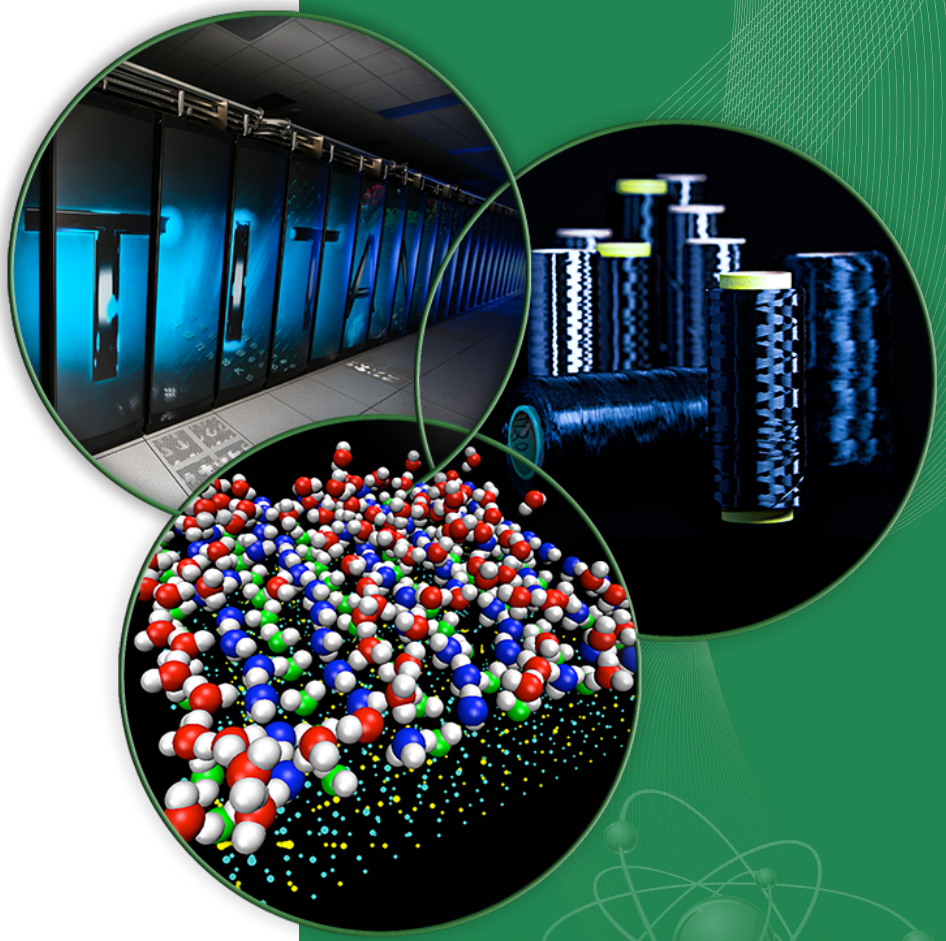


Cross Section Evaluation Working Group,
U.S. National Nuclear Data Week 2015
BNL, November 2-6, 2015

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory

Overview

- Integration into SCALE SQA
- Supported platforms
- New Features
  - SAMINT
  - New detector resolution functions

Integration into SCALE SQA:

- Version control of source code and test cases using Mercurial
- Bug tracking and workflow
- Cmake: auto configuration build (make –j)
- 25 executables built automatically on several platforms
- Ctest: auto testing tool
  - Test whether result are within a prescribed tolerance (1E-4)
    - SAMMY files tested: LST, PAR, LPT…
    - Makes it much easier to notice discrepancies.
  - 178 test cases from SAMMY 8.0.0 and
  - 4 new test cases for SAMINT
  - 1 new test case for RPI Lithium Glass detector resolution function
  - (All test cases include subcases.)

Supported platforms

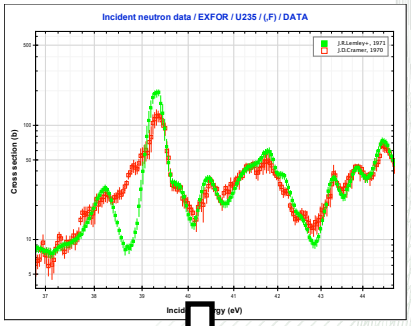
- Mac: gfortran
- Linux: gfortran, ifort
- Windows: ifort
  - Revealed few remaining issues that were corrected

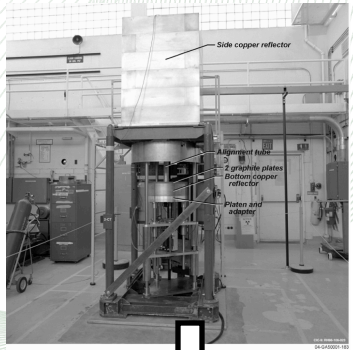
SAMINT: Nuclear Data Adjustment Based on Integral Experiments

- SAMINT is an auxiliary program designed to allow SAMMY to adjust nuclear data parameters based on integral data.
- Allow coupling of differential and integral data evaluation in a continuous-energy framework
- Update the parameters of a resolved resonance region evaluation directly based on integral benchmark experiments
- http://www.osti.gov/scitech/biblio/1185560/

Integral Experiments to Aid Nuclear Data Evaluation

- SAMINT can be used to extract information from integral benchmarks to aid the nuclear data evaluation process.
- Near the end of the evaluation based on differential experimental data, integral data can be used to:
  - Resolve remaining ambiguity between differential data sets
  - Guide the evaluator to troublesome energy regions
  - Inform the evaluator of the most important nuclear data parameters to integral benchmark calculations
  - Improve the nuclear data covariance matrix evaluation





SAMMY

ENDF

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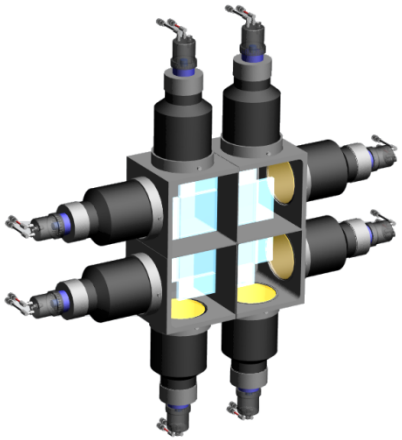
SAMINT Release Through RSICC

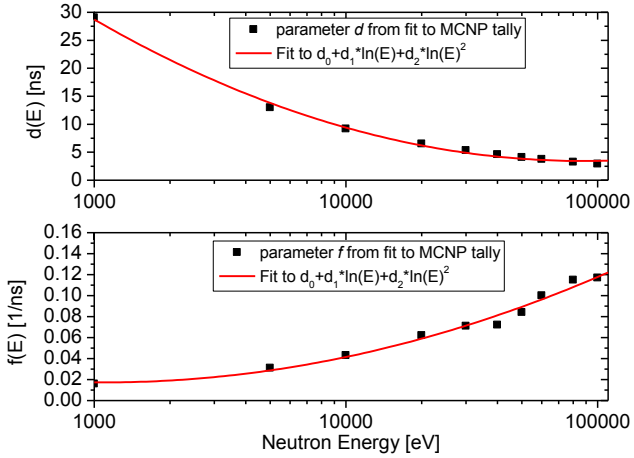
- SAMINT will now be distributed with the SAMMY code from RSICC! https://rsicc.ornl.gov/
- Optional, compile-time inclusion
- All linear algebra using LAPACK/BLAS
- Mac, Linux, Windows
- Version control

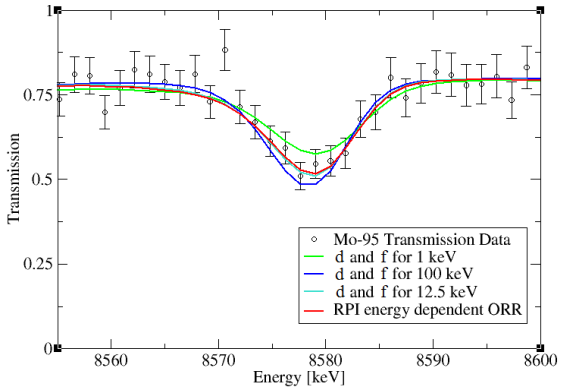
Case Name	SAMINT Capability	Sensitivity Code	Notes
tr181	- Resonance Parameter updating - Eta updating with correlations - Eta updating without correlations - Integral experiment covariance matrix	CE TSUNAMI-3D	Independently confirmed by MATLAB calculations
tr182	- ^{56}Fe case - Fitting resonance parameters with inelastic channel open	MCNP6	Compilation comes form appearance of zero cross-sections due to threshold reactions
tr183	- ^{239}Pu case - Fitting resonance parameter and nu-bar simultaneously - Independent eta updating	MCNP6	

^{6}Li-glass Neutron Detector Array MELINDA

- Improved parameterization
  - Based on MCNP simulations by Amanda Youmans (RPI)







Comparing the original SAMMY detector resolution function to the modified function with Mo-95 data

Before:

$$I(l) = \begin{cases} Dg & for\ 0 < t < d \\ De^{-f(t-d)} & for\ d < t \end{cases}$$

After:

$$d(E) = d_0 + \ln(E) * (d_1 + d_2 * \ln(E))$$

$$\boldsymbol{f(E) = f_0 + \ln(E) * (f_1 + f_2 * \ln(E))}$$

Liquid Scintillator Detector liquid $CH_{1.212}$

- Based on MCNP simulations by Amanda Youmans (RPI)

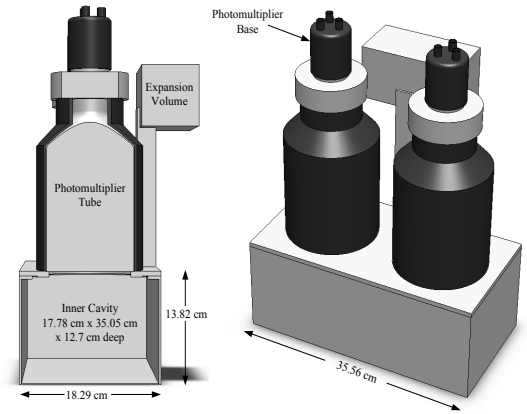
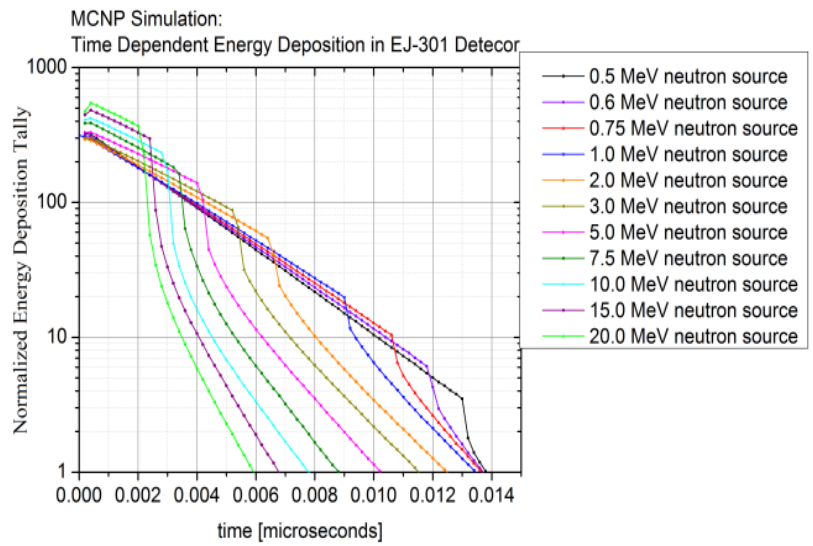
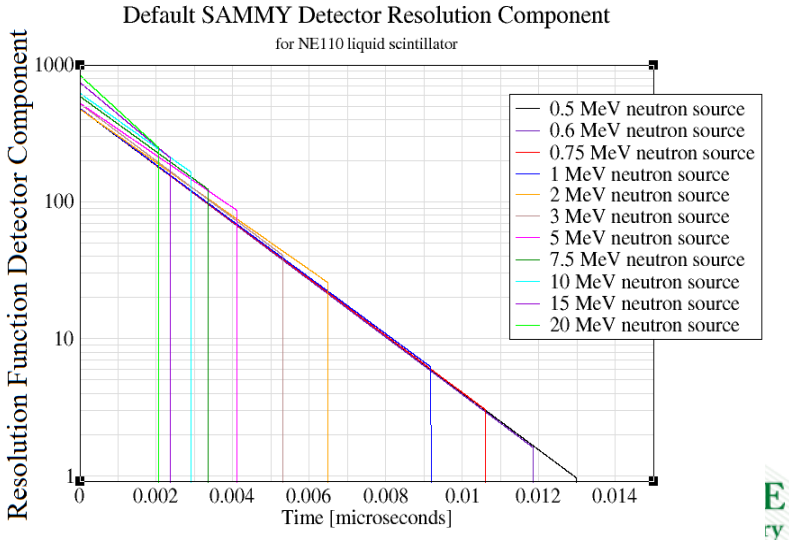


Table IV: Cross Sections for EJ-301 SAMMY Input	
Energy [eV]	Cross section [b]
500,000	7.967348
600,000	6.963397
750,000	5.958675
1,000,000	4.953201
2,000,000	3.101132
3,000,000	2.329274
5,000,000	1.683733
7,500,000	1.554593
10,000,000	1.172541
15,000,000	0.877705
20,000,000	0.663136





Minor upgrades

- Updated physicals constants
  - Consistent with SAMRML
  - SAMMY and SAMRML yield identical results now
- Corrected a misplaced index causing incorrect matrix multiplication for non-diagonal data covariance matrix
  - (uncovered and corrected by Vlad Sobes)
- Several other minor bug fixes
  - Revealed by compiler or platform idiosyncrasies

Conclusions and outlook

- SAMMY is well positioned for
  - further modernization
  - new feature development
    - Including in the URR
  - integration and code sharing with AMPX modules
    - e.g. SAMRML has been implemented in C++ by Andrew Holcomb

2016 R-Matrix Workshop

from June 27, 2016 to July 1, 2016 (US/Central) *Santa Fe, NM, USA*
US/Central timezone

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Main
Scientific Program
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Registration Form
List of registrants
Important Dates
Accommodations
Travel

✉ Support

Greetings R-matrix enthusiasts,

We would like to invite you to participate in a JINA-CEE sponsored workshop on all things R-matrix that will be held **June 27 to July 1, 2016,** in Santa Fe, New Mexico, USA.

The workshop will host a number of discussion topics covering experimental, application, and theoretical developments of R-matrix. The aim of the workshop is to bring together a diverse group with representatives from experiment and theory who utilize the R-matrix formalism for a variety of purposes. Sessions will be divided into different specialty topics ranging from nuclear astrophysics applications to mathematical theory to data evaluations. A major goal of the workshop will also be to compare different implementations of the theory in analysis codes and discuss different uncertainty analysis methods. While the workshop is largely targeted at specialists in the field, researchers from astrophysics or other applications that use nuclear physics inputs, as well as students and post-docs, are also highly encouraged to attend.

Organizing committee:

(Richard) James deBoer (co-chair, UND)
Mark Paris (co-chair, LANL)
Goran Arbanas (ORNL)
Carl Brune (OU)
Gerry Hale (LANL)
Ian Thompson (LLNL)
Ethan Uberseder (TAMU)
Morgan White (LANL)

We acknowledge support from Los Alamos and Oak Ridge National Laboratories, JINA-CEE, the University of Notre Dame, and the Institute of Nuclear and Particle Physics at Ohio University.

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https://indico.fnal.gov/conferenceDisplay.py?confId=10228

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Auxiliary slides

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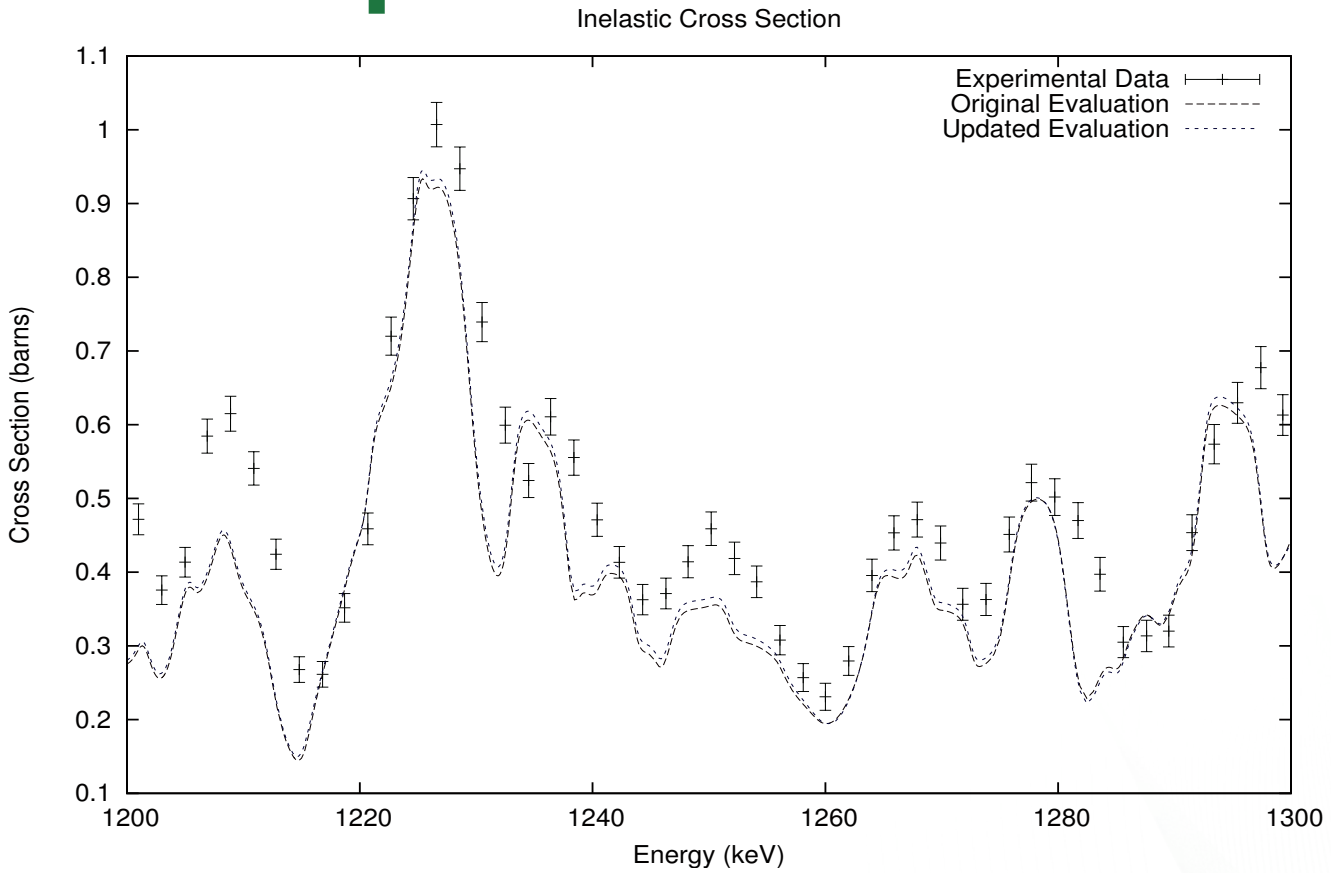
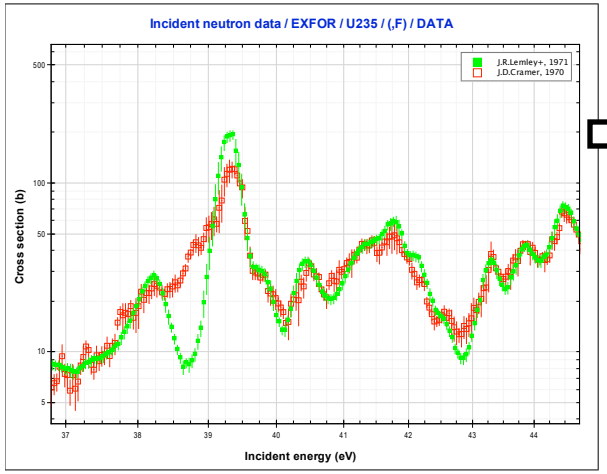
Cross Section Changes: Finer Scale than Differential Experimental Data



Inelastic cross section of ^{56}Fe before (χ^2 = 23.6023) and after (χ^2 = 22.9036) the adjustment based on integral experimental data plotted on top of differential experimental data of Perey, presented with one standard deviation error bars.

Using SAMINT with SAMMY

Differential Experimental Data



Integral Experimental Data

SAMMY

dσ(E)/dP

SAMINT

dk/dP

SAMMY

Updated P and δP

ENDF

dk/dσ(E)

CE TSUNAMI
MCNP-6

P stands for all resonance parameters: E_λ, Γ_γ , Γ_n , Γ_f , etc.