SAMMY Modernization

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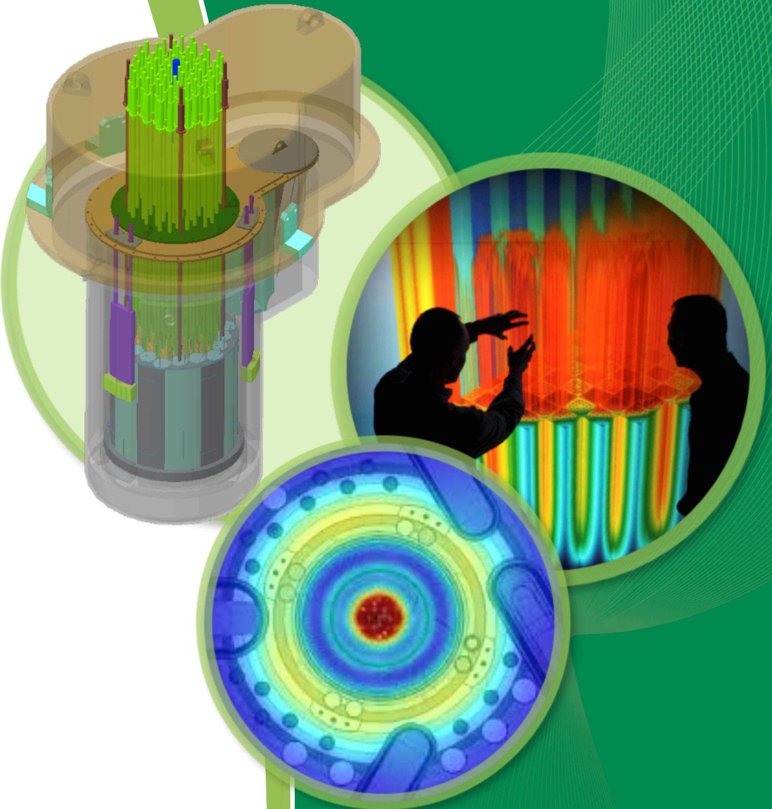

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Outline

- SAMMY history and overview of features
- SAMMY modernization update
  - SAMMY 8.1 release
  - Modernization strategy
  - Example: Coulomb functions
- SAMMY future directions
  - Simultaneous optimization of thermal and resolved R-matrix
  - Bayesian generalized data optimization for defective models
  - Generalized Reich-Moore approximation
- Summary and outlook

History of SAMMY

- Developed by Dr. Nancy Larson since 1970s
- 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
- 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: ORELA, RPI, GELINA
  – 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
- Charged projectiles (p, α)
- Unresolved resonance range (FITACS by F. Froehner)

Example SAMMY evaluation: Ti-48

- From: Leal, Luiz C., Guber, Klaus H., Arbanas, Goran, Wiarda, Dorothea, Koehler, Paul Edward, & Kahler, A. “Resonance Evaluation of ^{48}Ti Including Covariance for Criticality Safety Applications.” *ICNC 2011: 9th International Conference on Nuclear Criticality Safety,* United States

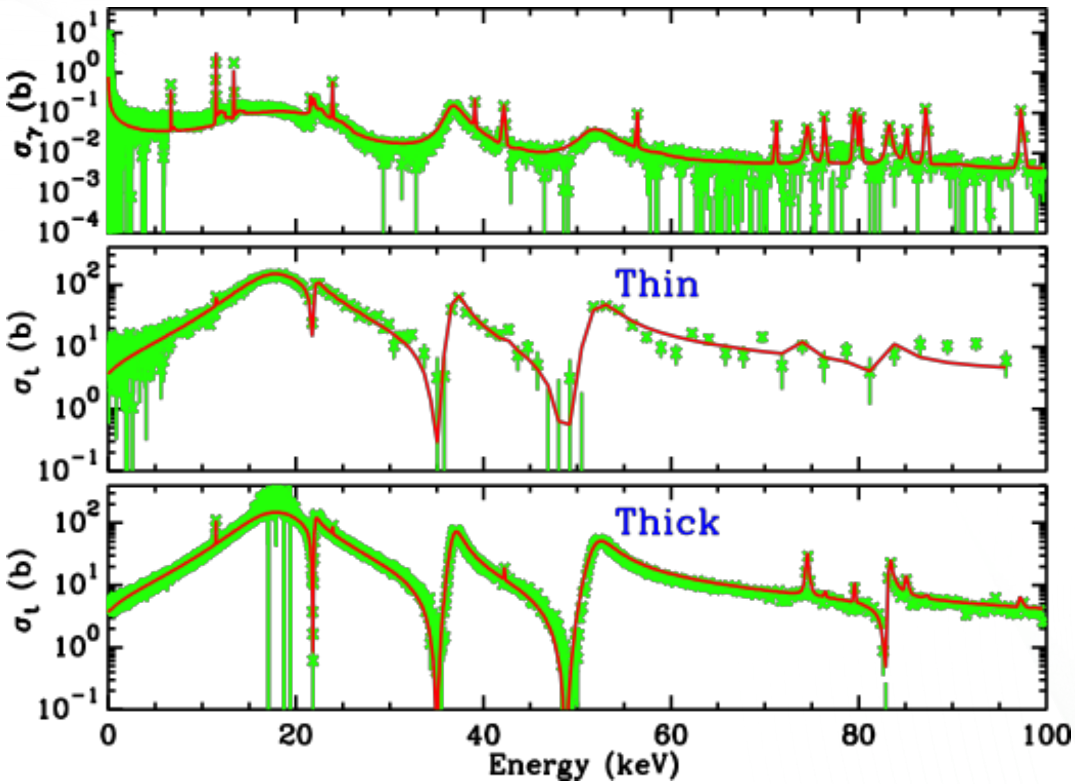

Figure 1. Comparison of the total (two transmission data) and capture cross section calculated in the energy range 10 eV to 100 keV with the resonance parameters and the experimental data for ^{48}Ti.

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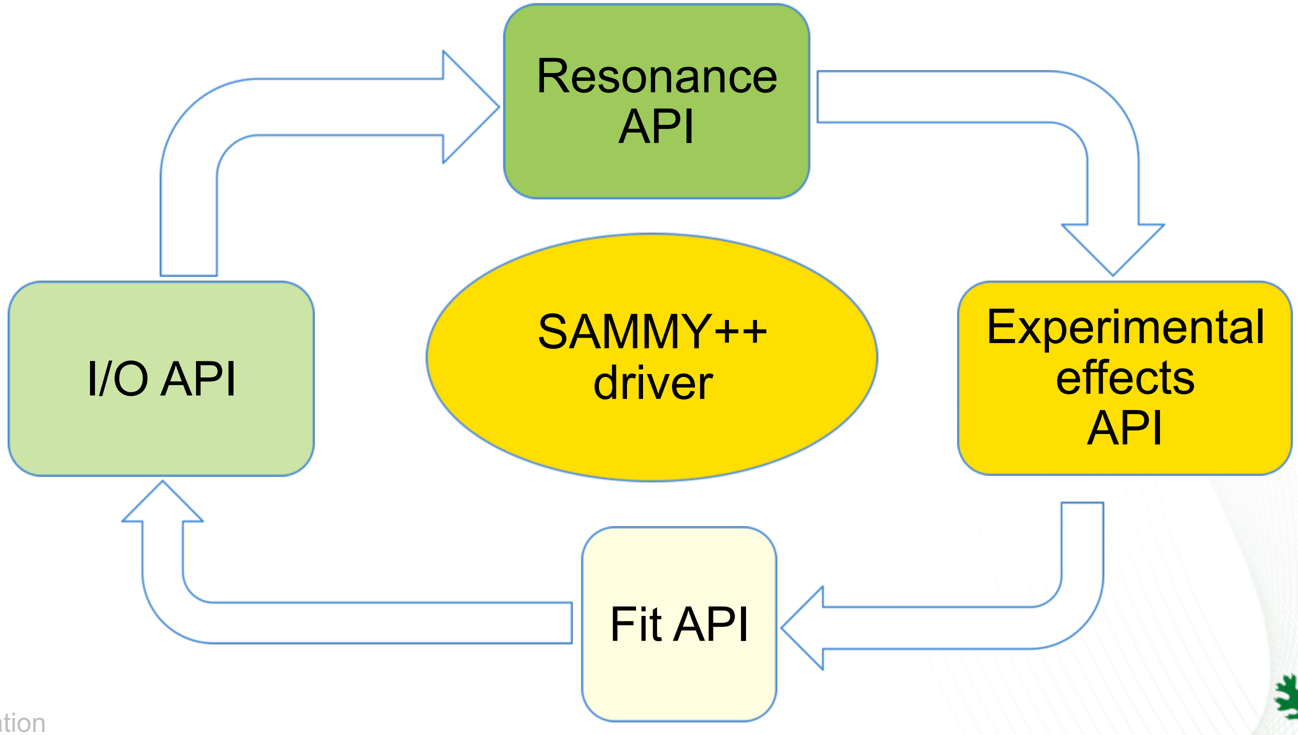
SAMMY 8.1 released by RSICC April 2017:

- 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 test cases

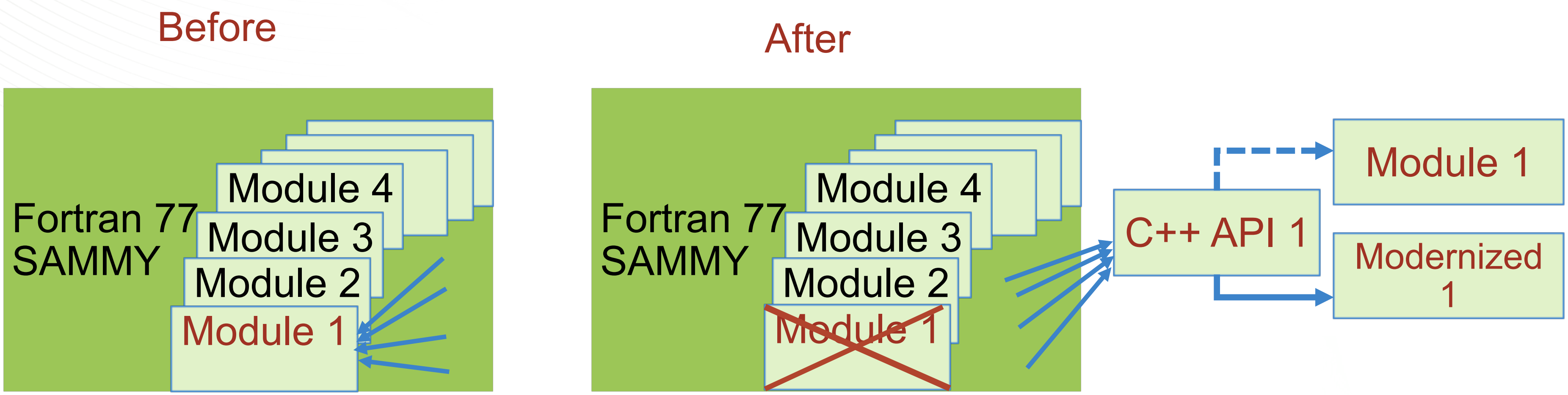
SAMMY++ high-level application programming interface (API) design

- Defines APIs before implementation
  - Enables interchangeable implementations for each API
  - Leverages input/output (I/O) and resonance API in modernized AMPX
    - SAMMY parameter and GND file reader/writer under development
    - Will replace SAMMY I/O routines



Modular modernization of SAMMY using APIs

Schematic diagram of SAMMY Fortran 77 legacy module modernization



Example: 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](https://doi.org/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 (next); enables conversion from R-matrix parameters to (and back) the Brune's alternative R-matrix, or the S-matrix poles, also known as Hwang "multipole" representations

Modernization of SAMMY methods

- **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	Generalized Reich-Moore approximation

Simultaneous evaluation of S(α,β) and RRR

- **Problem:** S(α,β) and RRR are evaluated *separately* by different evaluators/ codes
  - Covariance between the two is absent; may lead to discontinuity at the interface
  - Caused by distinct physical theories and codes used in respective evaluations
- **Solution:**
  - Develop S(α,β) expertise (C. Chapman) and couple with RRR expertise at ORNL
  - Relate parameters in S(a,b) and RRR and evaluate simultaneously
  - Coding is required to interface the optimization code to the S(a,b) and RRR codes
- **Benefits:**
  - Consistent evaluations of S(α,β) and RRR, including cross-covariances
  - Thermal S(α,β) cross sections include T-effects cf. conventional Doppler broadening
  - Similar problems exist at the interface of RRR and URR

Scattering length for S(α,β) and RRR

- This expression relates the bound scattering length used in S(α,β) evaluations to SAMMY RRR R-matrix parameters

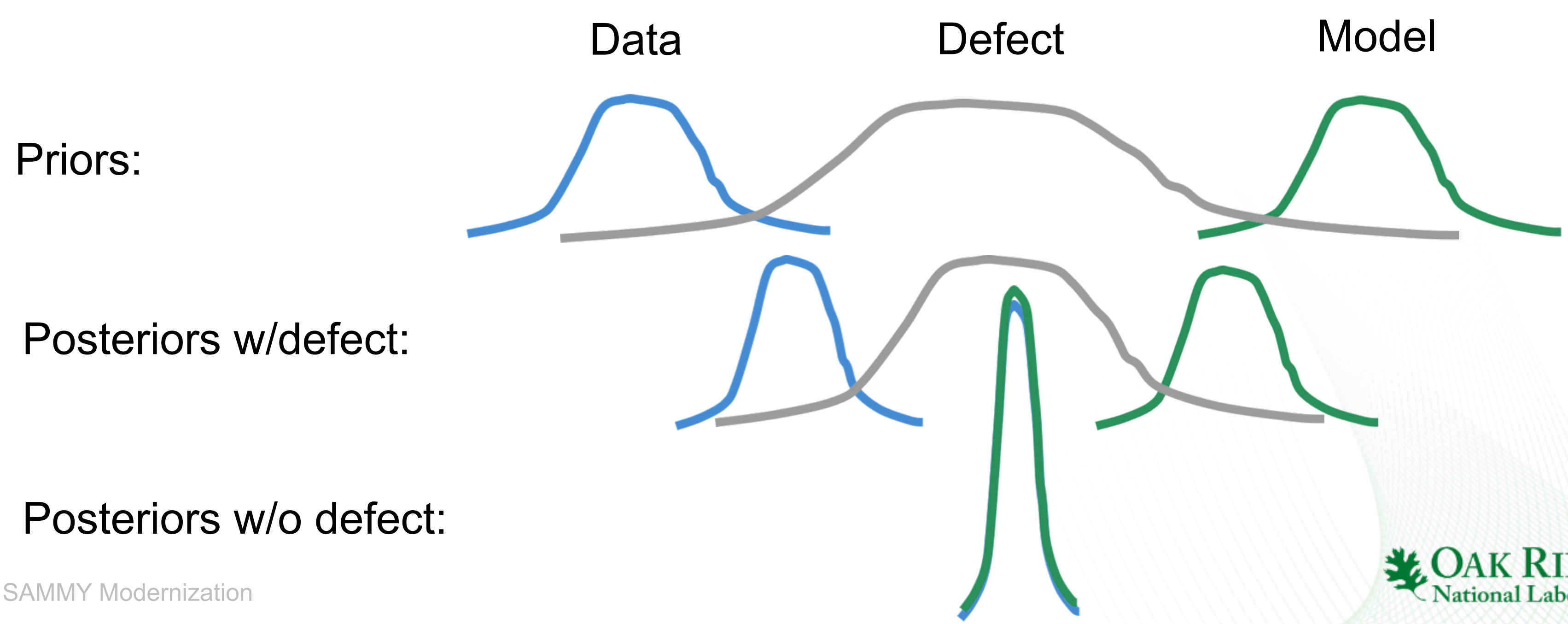
$$b(E) = \frac{A+1}{A} a(E)$$

$$a(E) = a_{s\text{-wave}}(1 - R_\infty - \frac{\gamma_{1s}^2}{E_1 - E - i\Gamma_{1\gamma}/2 - ik\gamma_{1s}^2})$$

- A Spallation Neutron Source proposal has been submitted to measure U_3O_8
- Complex scattering lengths model thermal neutron absorption

Bayesian optimization of *defective* models

- **Background:** Bayes theorem takes *prior* information about model parameters and data to yield *posterior* probability distribution functions
- **Problem:** Nuclear data evaluations assume perfect cross section models;
  → this assumption may yield incorrect posterior values and uncertainties
- **A solution:** Formally introduce model defect into the Bayes' theorem
- **Benefits:** Provides a Bayesian framework for model defects; posterior data values are no longer forced to equal posterior model prediction



Bayesian optimization of *defective* models

- Comparison to the conventional chi^2 minimization method:

Cost function (chi^2):

$$Q(z) \equiv (z - \langle z \rangle)^\intercal \mathbf{C}^{-1} (z - \langle z \rangle)$$

Constraint:

$$T(P) - D = \boxed{\delta}$$

where generalized data includes defect:

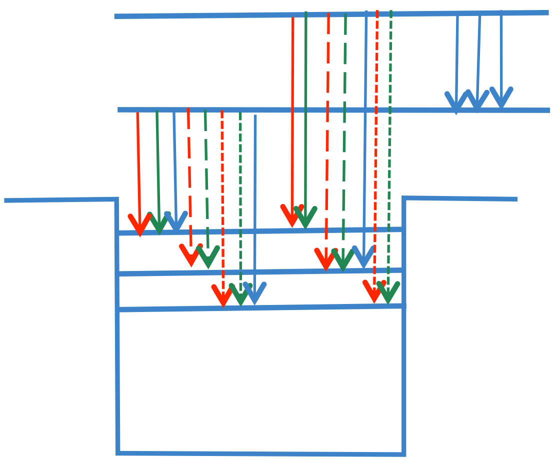
$$z \equiv (P, D, \boxed{\delta}) \qquad \langle z \rangle \equiv (\langle P \rangle, \langle D \rangle, \langle \boxed{\delta} \rangle)$$

$$\mathbf{C} \equiv \langle (z - \langle z \rangle)(z - \langle z \rangle)^\intercal \rangle \equiv \begin{pmatrix} \mathbf{M} & \mathbf{W} & \mathbf{X} \\ \mathbf{W}^\intercal & \mathbf{V} & \mathbf{Y} \\ \mathbf{X}^\intercal & \mathbf{Y}^\intercal & \mathbf{\Delta} \end{pmatrix}$$

G. Arbanas et al. (CW2017)

Generalized Reich-Moore approximation

- γ-ray channels
  - Defined by EM multipolarity, helicity, and final state quantum numbers
  - Selection rules based on final state quantum numbers, γ-ray multipolarity
  - Electric: E1, E2, E3 …
  - Magnetic: M1, M2, M3 …
- Level-level interference takes place via identical γ-ray channels



G. Arbanas, V. Sobes, A. Holcomb, P. Ducru, M. Pigni, and D. Wiarda (ND2016), *EPJ Web of Conferences* **146**, 12006 (2017) https://doi.org/10.1051/epjconf/201714612006

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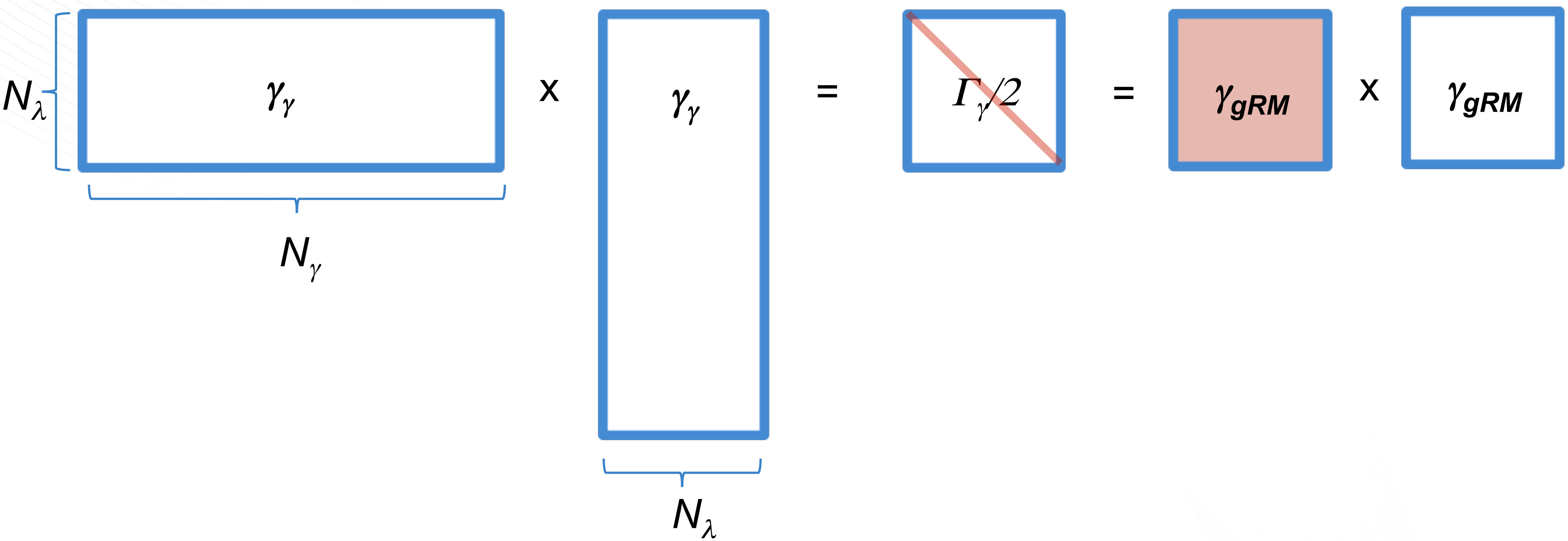
Generalized Reich-Moore approximation

- Consider capture-width parameter matrix for $N_\lambda << N_\gamma$:



- Since *total capture* cross section depends on Γ_γ, it could be fit equally as well by N_λ as it could by all N_γ capture channels, which is true for *total* capture only (individual γ-channels require full *R*-matrix)

Summary and outlook

- SAMMY 8.1 released in 2017
- SAMMY is under the SCALE SQA framework
- Modernization proceeds via API framework, including Coulomb functions, optimization…
- Code sharing with AMPX/SCALE (D. Wiarda, A. Holcomb) guarantees consistency and is conducive to new data formats
- Potential improvements to evaluation methods have been identified
  - Simultaneous evaluation of thermal and resolved resonance ranges
  - Generalized Reich-Moore approximation
  - Optimization of defective models
- Open source SAMMY is in progress, as well as AMPX (like NJOY), to enlarge developer/user base
- SAMMY 8.2 is expected later in 2018

Special thanks to SAMMY contributors

- Andrew M. Holcomb (ORNL)
- Dorothea Wiarda (ORNL)
- Marco T. Pigni (ORNL)
- Vladimir Sobes (ORNL)
- Christopher W. Chapman (ORNL)

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Auxiliary slides

Fit API: Preliminary interface

Interface
Fit
setData Set an instance of Data interface **initialize** After setting data object initialize internal data structures **execute** Do the actual fitting **finalize** Clean up any internal resources

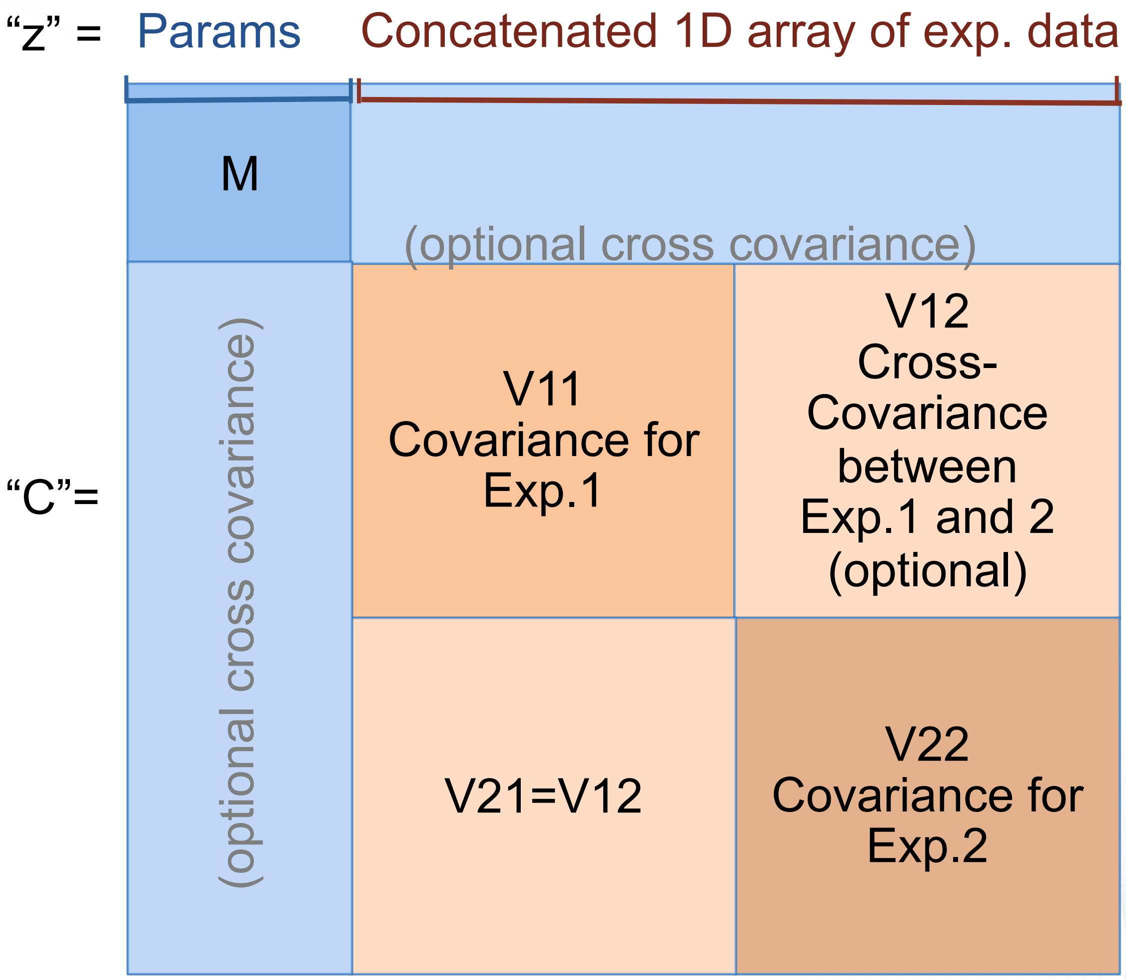
Interface
Array
getNumDim Get the number of dimensions **getSize(int dim)** Get the array size for dimension m **getValue(int i1, int i2, …)** Get the value for the indicated indices. In C++ we would pass in a vector of length getNumDim **setValue(int i1,int i2, …_** Set value

Interface
Data
getNumberParams Get the number of parameters **getNumData** Get the number of experimental data **getData** Get the list of experimental data (1-dim Array) **getParam** Get the list of initial params (1-dim Array) **getCovMatrix** Get the full covariance matrix (2-dim Array) **getTheory** Get theoretical values based on current parameters (1-dim Array) **setParam** Set the current parameters (1-dim Array) **setCovMatrix** Set the full covariance matrix (2-dim Array)

- Actual instances are instantiated by a factory class
- Data will have a method to obtain the derivatives (2-dim Array: getNumberParams x getNumData); there will be a function that computes derivatives numerically
- Fit calls setParams, getTheory, setCovMatrix repeatedly in the course of fitting the data

Fit API: GLS implementation

- Parameters and experimental data cast into 1D array by implementation of data
  - for generic use inside SCALE framework
  - Froehner's formulation and notation:



Fit API: GLS, Bayesian Monte Carlo

GLS

Bayesian Monte Carlo

- Generalized least squares (GLS)
  - Nuclear Engineering Science Laboratory Synthesis (NESLS) summer intern Jinghua Feng implemented a prototype
  - Andrew Holcomb ported the prototype into the FitAPI
- Implementation uses *cpp-array* library (CPC **185**,1681, 2014)
  - Transparently parallelized via BLAS library (Intel MKL)
  - Compact expressions implemented directly (Sect. 2.2, JEFF Report 18, 2000)
- BLAS speeds up large matrix operations in SAMMY and shortens code
  - Arbanas, Dunn, Wiarda, M&C2011, http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/47/073/47073019.pdf

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Experimental effects (EE) API

- Convolution of Doppler broadening, target, and detector effects, each one implenting the EE API:

Doppler broadening:
FGM, DDXS, S(a,b)
BROADEN/AMPX

Neutron transport:
SHIFT API

- SHIFT API for on-the-fly neutron transport aspects
  - To enable fitting integral benchmark experiments (IBEs)
  - Developed for SCALE by Cihangir Celik in FY2017
  - Message passaging interface (MPI) enabled
  - Could use MCNP input
- In principle, the entire experimental setup could be simulated; fitting to raw data may be desirable to avoid PPP; varying opinions

Modular modernization of SAMMY using APIs

For each SAMMY Fortran 77 legacy module to modernize:

1. Create a layer of indirection to the module by designing its C++ API
2. Move the module out of SAMMY and use it to implement its C++ API
3. Redirect all module calls to the C++ API implementation outside SAMMY and then re-run SAMMY test cases and correct any problems until identical results are reproduced
4. Implement the C++ API using a modernized code or a third-party library
5. Recompile SAMMY with the modern implementation of the C++ API and then re-run SAMMY test cases and re-baseline the results when justified

Phenomenological Dirac R-matrix formalism

- Originally derived for calculable R-matrix, but expressed in a form that could be used for phenomenological fitting:
  PhD Thesis (2011): http://scholarworks.wmich.edu/dissertations/411
- Boundary condition is determined by the channel radius
- Compare to approximations and the nonrelativistic R-matrix

J. Grineviciute and Dean Halderson, *Physical Review C,* **85,** 054617 (2012)

$$R_{cc'} = \sum_{\mu} \gamma_{\mu c}\gamma_{\mu c'}/(E_\mu - E)$$

$$\mathbf{S} = \mathbf{v}^{1/2}(\mathbf{Fo} - \mathbf{RGo})^{-1}(\mathbf{F_I} - \mathbf{RG_I})\mathbf{v}^{-1/2} \qquad T_{cc'} = i(\delta_{cc'} - S_{cc'})/2$$

$$\langle f \rangle_{\alpha\sigma M_A,\alpha'\sigma' M'_A} = \frac{1}{k} \sum \sqrt{4\pi(2\ell+1)} C^{\ell 1/2 j}_{0\sigma m} C^{J_A j J_B}_{M_A m M_B} C^{J'_A j' J_B}_{M'_A m' M_B} C^{\ell' 1/2 j'}_{m'_\ell \sigma m'}$$
$$\times i^{(\ell-\ell')} e^{i(\delta'_\kappa + \delta'_{\kappa'})} T_{\alpha J_A \ell j J_B, \alpha' J'_A \ell' j' J'_B} Y_{\ell' m'_\ell}(\mathbf{k}').$$

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{2(2J_A+1)} \sum_{\sigma\sigma' M'_A M'_A} \left| \langle f_c \rangle_{\sigma\sigma'} \delta_{J_A \alpha M_A, J'_A \alpha' M'_A} + \langle f \rangle_{\alpha\sigma M_A,\alpha'\sigma' M'_A} \right|^2$$

ORNL S(a,b) evaluation framework overview

- The objective is to combine experimental double differential scattering data and model parameters to yield the best estimate of double differential cross section (DDCS) and ***uncertainties***
- Data and simulation fit is achieved using the unified Monte Carlo (UMC) [1] method
- Simulations are constrained by physical properties of material
- Framework is tested on light water
  - Data collected from ORNL SNS
  - Rensselaer Polytechnic Institute (RPI) collaboration
- Validated using benchmarks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook
- C. Chapman's Ph.D. https://smartech.gatech.edu/handle/1853/58693