

SAMMY: an ORNL Tool for Generating Covariance Matrices in the Resonance Region

**Workshop on Nuclear Physics and Related
Computational Science R&D for Advanced Fuel Cycles**

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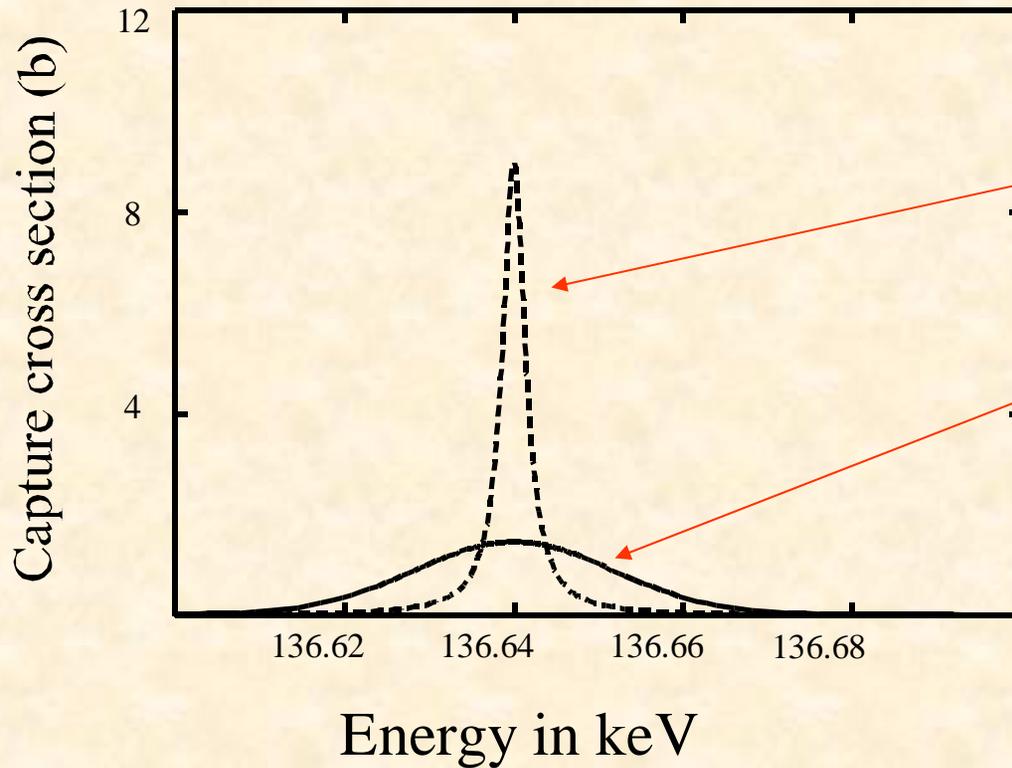
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Measured data cannot be used directly for integral calculations

- **Each type of data comes from a separate measurement** capture, total, fission, reaction, etc.
 - However, the various types are highly interrelated
- **Data include measurement-related effects**
 - Finite temperature
 - Finite size of samples
 - Finite resolution
 - Other machine-dependent features
 - Measured data may look very different from the underlying “true” cross section as shown on next slide

Doppler broadening only ...



Capture cross section for ^{58}Ni without Doppler broadening (dashed curve) and with Doppler broadening at 300 K (solid curve)

Advantages of evaluated data --

- **Incorporate theoretical understanding**
 - Cross section shapes
 - Relationships between cross sections for different reactions
- **Incorporate all available experimental data and all available uncertainty information**
- **Allow extrapolation**
 - Different temperatures
 - Different energies (lower, higher, in-between)
 - Different reactions

RRR evaluations are done with SAMMY

- **SAMMY is used to analyze measured data and produce evaluations**
- **Developed at ORNL, used at ORNL and around the world for analysis of neutron-induced cross sections**

also can be used for charged-particle evaluations

RPI, KAPL, LANL, TUNL, nTOF, CEA, GELINA, ...

- **Uses multilevel multichannel R-matrix**
- **Includes corrections for experimental conditions**

Doppler, resolution, multiple scattering, normalization, background ...

SAMMY (cont.)

- Capable of efficient handling of full off-diagonal covariance matrix for experimental data
- Produces full off-diagonal resonance parameter covariance matrix = RPCM
- Creates ENDF File 2 and File 32

Main topics for
this presentation

Two methods for generating RPCM

- **Customary method, used for new evaluations**

- RPCM is generated by the **fitting procedure** automatically

Bayes' method = generalized least squares

- Incorporates all experimental uncertainties

to the extent that the analyst provides the input information

- **Retroactive method, used when a new evaluation is not possible**

- ENDF File 2 exists but File 32 is empty.
- Time and manpower are not immediately available for a complete new evaluation.
- Users do not want new evaluations unless and until they are necessary.

SAMMY's retroactive RPCM method

- 1. Generate artificial “experimental” data from ENDF resonance parameters**
 - Capture, fission, total, whatever
 - Include Doppler and resolution broadening, other experimental effects as appropriate
- 2. Make reasonable assumptions regarding experimental uncertainties**
 - **Statistical** diagonal contribution to data covariance matrix
 - **Systematic** off-diagonal contribution to data covariance matrix
 - **Normalization, background, broadening, etc.**

Retroactive RPCM, continued

- 3. Prepare SAMMY runs in which all important resonance parameters are varied**
- 4. Include systematic uncertainties for measurement-related quantities**
 - Normalization, background, broadening, etc.
- 5. Perform simultaneous fit to all the data**
 - All “experimental uncertainty” is thereby propagated to the RPCM

**PUP = Propagated Uncertainty Parameter
= contributor to data covariance matrix**

Retroactive RPCM, continued

6. Consider the output:

- **Parameter values do not change very much**
- **Parameter covariance matrix is therefore a good approximation to the “correct” RPCM**

important



7. Write RPCM into ENDF File 32

Justification for retroactive method

- Consider least squares equations

A simplified form
of Bayes' method

$$P' = P + M' G^t V^{-1} (D - T) \quad M' = (G^t V^{-1} G)^{-1}$$

- If $D \approx T$ then $P' \approx P$, so M' is a good approximation for the RPCM for P

P = initial parameter values

P' = new parameter values

M' = new covariance matrix for parameters

T = theory

D = experimental data

G = sensitivities (partial derivatives)

V = covariance matrix for experimental data

There are challenges ...

- **Super-large cases require special care**
 - ^{235}U , for example, has
 - ~3000 resonances
 - 5 parameters for each resonance
 - **Not every computer can accommodate large cases**
 - large memory
 - long run time
 - **We are operating at the limit of our available computers!**

High-performance computers
would be a great asset for
these calculations!

Other challenges ...

- **Which contributors are important and which can safely be neglected?**

- **Also, which resonances?**

Normalization uncertainty?
Background uncertainty?
Resolution uncertainty?
Others?

- **Can methodology uncertainties be incorporated?**

- **For example**

- **R-matrix treats only compound effects (not direct)**
- **Multiple-scattering correction is imperfect**
- **Not all experimental uncertainties are known**
- **Some spin assignments are dubious**

Testing and correcting

- **At ORNL, after the RPCM is generated, integral tests are used to determine whether the RPCM leads to reasonable results**

- **AMPX code is used to process ENDF file (including File 32 via PUFF-IV) into multigroup cross sections and associated covariance matrix**
- **TSUNAMI module of SCALE code is used to calculate integral quantities with their associated uncertainties**

Mike Dunn will talk more about these later today

- **If uncertainties are deemed too small, they may be increased in the RPCM**

Evaluator may choose to increase uncertainties while keeping correlation coefficients the same.

ORNL contributions to ENDF/B-VII

- **Resonance parameters (File 2)**

- ^{233}U , ^{235}U , ^{238}U , ^{232}Th , ^{239}Pu , ^{240}Pu , ^{241}Pu

- ^{35}Cl , ^{37}Cl , ^{19}F , $^{28,29,30}\text{Si}$, ^{27}Al

currently pointwise cross sections

- **Covariance matrices (File 32)**

- ^{152}Gd , ^{154}Gd , ^{155}Gd , ^{156}Gd , ^{157}Gd , ^{158}Gd , ^{160}Gd

- ^{232}Th

Work in progress

CERN nTOF capture data has been measured; Spaniards are analyzing with SAMMY in consultation with Derrien and Larson

- **Resonance parameters plus covariances**

– ^{103}Rh , ^{239}Pu , ^{241}Pu , ^{55}Mn , ^{39}K , ^{41}K , ^{35}Cl , ^{37}Cl , ^{240}Pu

a few months

Work has started, but waiting for new data

Currently these are pointwise cs

- **Covariance matrices (File 32)**

– ^{235}U , ^{233}U , ^{238}U , ^{240}Pu , ^{19}F , $^{28,29,30}\text{Si}$, ^{27}Al

end of year

- **Future evaluations will include both File 2 and File 32**

Research and development opportunities

- **Additional research needed to understand and include methodology uncertainties**
- **Improve ENDF unresolved resonance region**
 - Format for File 2 is antiquated; collaborative effort is underway to improve this
 - ANL, ORNL, Europeans
 - File 32 developments await File 2 format developments
- **SAMMY improvements**
 - Modernization of matrix manipulation algorithms
 - Graphical user interface to be developed
 - New features? the wish list is long!

High-performance computers would help with large cases, for example ^{235}U , which must currently be analyzed piece-meal.

The End