Covariance and Sensitivity Data Generation at ORNL

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ICRS 10 RPS 2004

Madeira, Portugal
May 9-14, 2004

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

OUTLINE

- **Computer code SAMMY**
- **Covariance Generation Methodology**
- **Description of the Retroactive Covariance Generation Methodology**
- **Concluding Remarks**

COMPUTER CODE SAMMY

- **Used for analysis of neutron, charged particle cross- section data.**
- **Uses Bayes' method (generalized least squares) to find parameter values.**
- **Uses R-matrix theory, Reich-Moore approximation (default) or multi- or single-level Breit-Wigner theory.**
- **Generates covariance and sensitivity parameters for resolved and unresolved resonance region (generalized least squares).**

Average Group Cross Section

$$\Phi_g \overline{\sigma}_{xg} = \int_{E_g}^{E_{g+1}} \sigma_x(E)\Phi(E)\,dE$$

with

$$\Phi_g = \int_{E_g}^{E_{g+1}} \Phi(E)\,dE$$

Covariance Matrix for Group Cross Sections

If $p_1, p_2, \ldots, p_n$ are evaluated resonance parameters such that

$$\sigma_x = \sigma_x(p_1, p_2, \ldots, p_n)$$

Then

$$\delta\bar{\sigma}_{xg} = \sum_j \frac{\partial \sigma_{xj}}{\partial p_j} \delta p_j$$

Group Covariance Matrix

$$< \delta\bar{\sigma}_{xg} \; \delta\bar{\sigma}_{xg'} > = \sum_{j\,k} \frac{\partial\sigma_{xj}}{\partial p_j} < \delta p_j \; \delta p_k > \frac{\partial\sigma_{xk}}{\partial p_k}$$

Covariance of the group cross sections depends on the covariance of the resonance parameters *p as*

$$< \delta p_j \; \delta p_k >$$

These quantities are calculated in SAMMY and are stored in the ENDF library

Cross Section Energy Ranges

- **In general, in the Evaluated Nuclear Data Files (ENDF), the neutron cross sections representation are given for three energy regions:**

  Resolved: from low energy up to ~ 1 MeV

  Unresolved: from 1 MeV to ~5 MeV

  High Energy: above 5 MeV

- **Computer Code SAMMY is used to evaluate cross sections and generate covariance data in the RESOLVED and UNRESOLVED energy regions**

ENDF Covariance Representation (resonance parameters)

- **Resolved Resonance Region**

File (MF) 2 Section (MT) 151 contains

R-Matrix Resonance Parameters

Formalism most used in ENDF/B-VI is based in the Reich-Moore (RM) methodology

Resonance Parameters in the RM formalism

$$E_r \quad \Gamma_\gamma \quad \Gamma_n \quad \Gamma_{f1} \quad \Gamma_{f2} \text{ etc.}$$

ENDF Covariance Resonance Representation

- **Covariance of Resolved Resonance Parameters**

File (MF) 32 Section (MT) 151

$(\delta E_r)^2$ Resonance energy variance

$(\delta \Gamma_\gamma)^2$ Gamma Width variance

$(\delta \Gamma_n)^2$ Neutron Width variance

$(\delta \Gamma_{f1})^2$ Fission Width variance (channel one)

$(\delta \Gamma_{f2})^2$ Fission Width variance (channel two)

$(\delta \Gamma_n \delta \Gamma_\gamma)$ Covariance of Γ_n and Γ_γ

$(\delta \Gamma_n \delta \Gamma_{f1})$ Covariance of Γ_n and Γ_{f1}

$(\delta \Gamma_n \delta \Gamma_{f2})$ Covariance of Γ_n and Γ_{f2}

ENDF Covariance Resonance Representation

- **Unresolved Resonance Region**

File (MF) 32 Section (MT) 151

Cross section representation:

Single-Level Breit-Wigner

$$\langle D \rangle \quad \langle \Gamma_\gamma \rangle \langle \Gamma_n \rangle \quad \langle \Gamma_f \rangle \quad \langle \Gamma_x \rangle \text{ etc}$$

Covariance also given in FILE 32

Covariance Processing Tools

- **NJOY**
  - **Not capable of processing RM covariance data**
- **PUFF**
  - **Not capable of processing RM covariance data**
- **ERRORJ**
  - **Process most of R-matrix covariance data**

Covariances in SAMMY Output

- **There exist two possible scenarios for generating covariance data in SAMMY**

  Direct result from the SAMMY data evaluation

  Automatically generated by every SAMMY fit of the experimental data

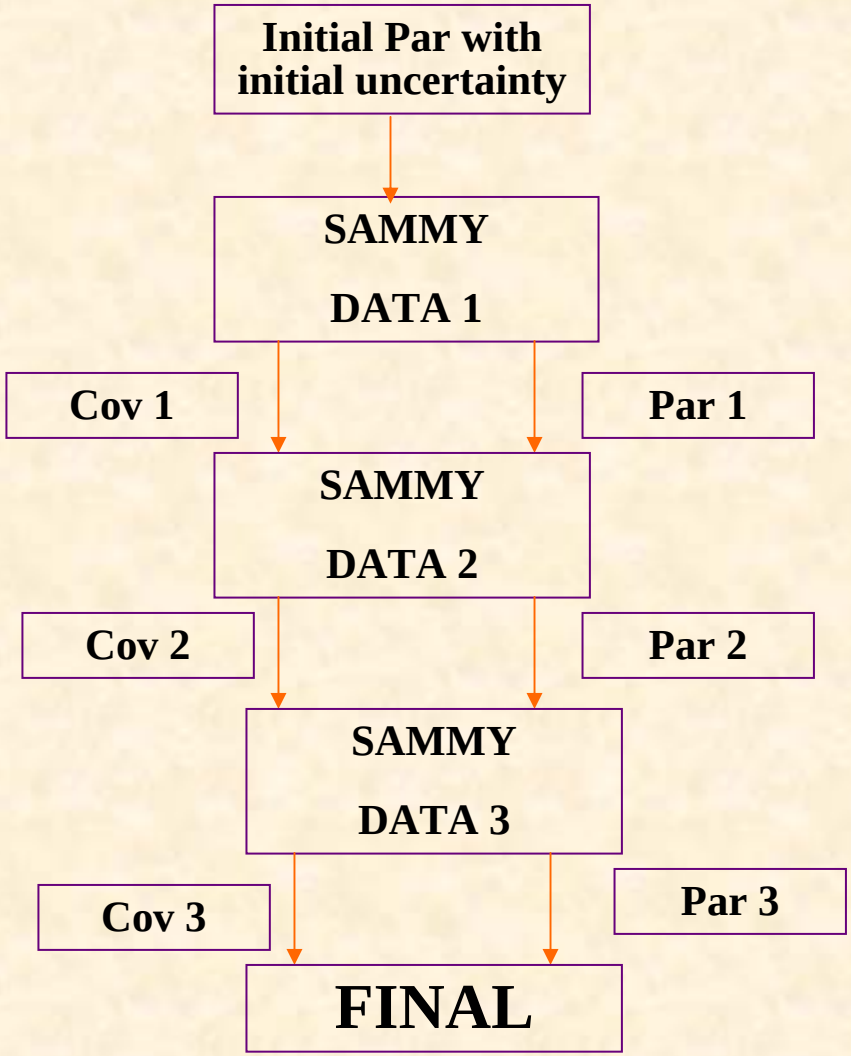
  Retroactively constructed covariance when the Data Evaluations Exist

  This is the approach used for generating covariance for gadolinium isotopes

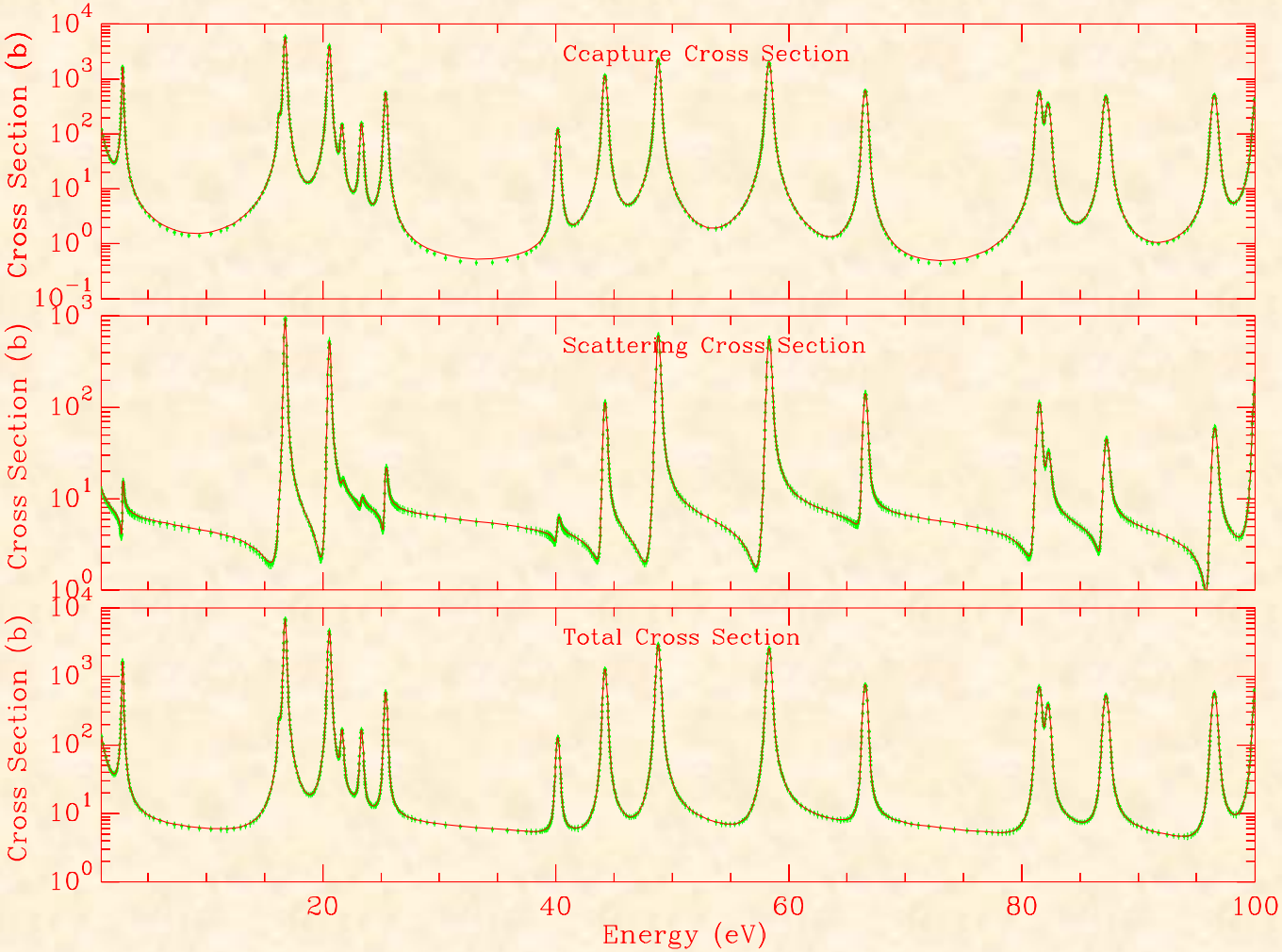
Retroactive Covariance Generation in SAMMY for Gadolinium

- Select the best available evaluation from the nuclear data libraries
- Convert the resolved resonance parameters from Multi-Level Breit-Wigner formalism to the Reich-Moore formalism
- Retrieve resonance parameter uncertainties from the literature
- Generate "experimental" cross section for total, scattering, and capture cross sections with NJOY code which will be used as "experimental data" in SAMMY
- Assign a global "experimental" uncertainty to the experimental data consistent with the evaluator's experiences with data analysis
- Run SAMMY code with the option to generate resonance-covariance retroactively
- Convert the resonance-covariance results from SAMMY into the ENDF format for file 32 (resolved and unresolved energy regions) and MT=151

Updated resonance parameter covariance



^{157}Gd Cross Sections from 1 eV to 100 eV



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

- **Resolved and Unresolved Resonance Evaluations Revised**
  - **MLBW resonance parameters converted to RM parameters**
  - **Unresolved resonance evaluation done with SAMMY: Average SLBW parameters obtained**
  - **SAMMY used to reevaluate the RM parameters**
- **Resolved and Unresolved Resonance Covariance Evaluation done with SAMMY**
  - **Uncertainty in the Resonance Parameters reported on "Mughabghab's Book" used as input**
  - **"Typical" data uncertainty on "data" were used. Example: ORELA resolution function, TOF uncertainties, channel widths, jitters, etc**
- **Use SAMMY Retroactive Scheme to Generate Covariance Data**

ERRORJ processing of ^{157}GD (44-group structure)

relative covariance (mt 1 , ig , mt 1 , igp) 584.3s

ig	igp	+0	+1	+2
1	1	2.233E-05		
2	2	2.224E-05		
3	3	2.263E-05		
4	4	2.447E-05		
5	5	2.907E-05		
6	6	3.107E-05		
7	7	3.192E-05		
8	8	2.912E-05		
9	9	2.806E-05		
10	10	3.488E-05		
11	11	4.966E-05		
12	12	5.460E-05		
13	13	5.651E-05		
14	14	5.791E-05		
15	15	5.931E-05		
16	16	6.039E-05		
17	17	6.083E-05		
18	18	6.114E-05		
19	19	6.149E-05		
20	20	5.945E-05		
21	21	4.880E-05		
22	22	4.481E-05		
23	23	4.858E-05		

ERRORJ processing of ^{157}GD (44-group structure)

...contribution from resonance parameters (mf=32)...

ig	igp	resolved	unresolved
1	1	2.233E-05	0.000E+00
2	2	2.224E-05	0.000E+00
3	3	2.263E-05	0.000E+00
4	4	2.447E-05	0.000E+00
5	5	2.907E-05	0.000E+00
6	6	3.107E-05	0.000E+00
7	7	3.192E-05	0.000E+00
8	8	2.912E-05	0.000E+00
9	9	2.806E-05	0.000E+00
10	10	3.488E-05	0.000E+00
11	11	4.966E-05	0.000E+00
12	12	5.460E-05	0.000E+00
13	13	5.651E-05	0.000E+00
14	14	5.791E-05	0.000E+00
15	15	5.931E-05	0.000E+00
16	16	6.039E-05	0.000E+00
17	17	6.083E-05	0.000E+00
18	18	6.114E-05	0.000E+00
19	19	6.149E-05	0.000E+00
20	20	5.945E-05	0.000E+00
21	21	4.880E-05	0.000E+00
22	22	4.481E-05	0.000E+00
23	23	4.858E-05	0.000E+00
24	24	5.439E-06	0.000E+00
25	25	3.169E-06	0.000E+00
26	26	2.883E-06	0.000E+00
27	27	1.675E-05	0.000E+00
28	28	9.108E-06	0.000E+00
29	29	7.049E-06	7.413E-06
30	30	0.000E+00	1.626E-05
31	31	0.000E+00	1.004E-05
32	32	0.000E+00	7.790E-06
33	33	0.000E+00	1.063E-05

Resolved

Unresolved

Concluding Remarks

- **Cross section and covariance evaluation in the resonance region were done for ^{152}Gd, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, and ^{160}Gd**
- **NJOY/AMPX were used to process the new evaluation;**
- **Covariance data were processed using the ERRORJ code;**
- **ERRORJ produces covariance data in the COVERX format;**
- **Application to benchmark calculations were done. Calculations were done with the TSUNAMI code**
- **Procedure will be used for other Isotope (actinides, fission products, structural material isotopes)**