Resonance Region Covariance Data for ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu

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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 resonance region.**

paradigm shift

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Covariances Generation with SAMMY

- **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 data**

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ENDF Covariance Representation
(resonance parameters)

- **Resolved Resonance Region**

File (MF) 2 Section (MT) 151 contains

     - R-Matrix Resonance Parameters

I   **- Formalism most used in ENDF/B-VII 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}**

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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

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

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 (FILE32)

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Averaged Group Cross Sections
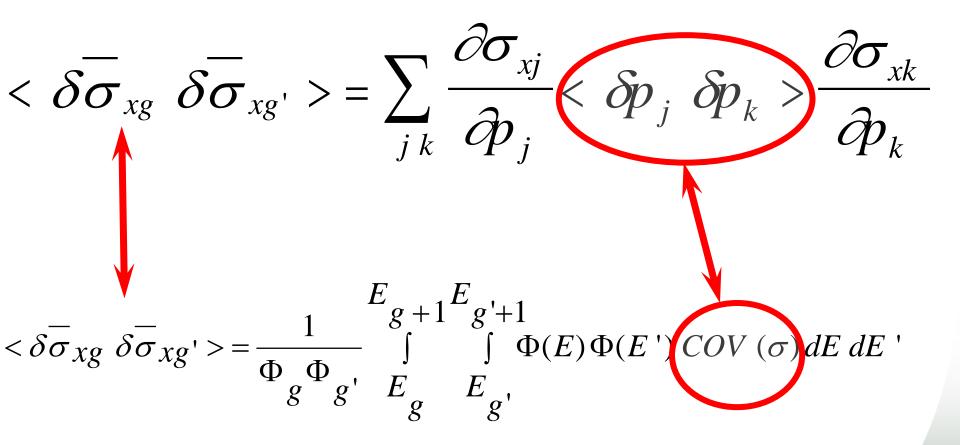
- **Alternatively, the group covariance cross section can also be obtained as**

$$< \delta \bar{\sigma}_{xg} \; \delta \bar{\sigma}_{xg'} > = \frac{1}{\Phi_g \Phi_{g'}} \int_{E_g}^{E_{g+1}} \int_{E_{g'}}^{E_{g'+1}} \Phi(E) \Phi(E') COV(\sigma) \, dE \, dE' \quad .$$

- *COV(σ)* **is the covariance representation for the pointwise cross section, that is, the ENDF FILE33 representation.**

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Question:
Can one find an equivalence ?

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

$$< \delta\bar{\sigma}_{xg} \ \delta\bar{\sigma}_{xg'} > = \frac{1}{\Phi_g \Phi_{g'}} \int_{E_g}^{E_{g+1}} \int_{E_{g'}}^{E_{g'+1}} \Phi(E)\Phi(E') \, COV(\sigma) \, dE \, dE'$$

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FILE32 to FILE33 Conversion

Procedure developed at ORNL:

Allows converting FILE32 covariance representation into FILE33

First Step: The task is to find an energy mesh that can be used to represent $COV(\sigma)$ such that the uncertainty in the group cross section reproduces that using the FILE32 representation;

Second Step: Generate FILE32 Covariance into the COVERX format using the PUFF-IV code;

Third Step: Use the COVCON code to convert COVERX into FILE33

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Application

- ^{233}U

- ^{235}U

- ^{238}U

- ^{239}P

Note:

^{232}Th (ORNL/IAEA) evaluation already in ENDF/B-VII done using the COMPACT FORMALISM (**LCOMP=2**)

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Covariance Evaluations for ^{233}U

- **Reich-Moore resonance evaluation in the energy range 0 to 600 eV;**

- **Total of 769 resonances including the external levels;**

- **Five parameters:**
  - Resonance energy E_r
  - Gamma width Γ_γ,
  - Neutron width Γ_n
  - Two fission widths Γ_{f1} and Γ_{f2}
  - Total of 3845 parameters;

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Covariance Evaluations for ^{233}U

- **"Retroactive" based on real experimental data**

- **Resonance Parameter Covariance Matrix (RPCM) generated**
  - **LCOMP=1 option**
  - **RPCM size of 100 megabytes (FILE32)**

- **Conversion from FILE32 into FILE33, i.e., Cross Section Covariance Matrix (CSCM)**
  - **329 energy boundaries used**
  - **CSCM size of 3 megabytes**

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Covariance Evaluations for ^{235}U

- **Reich-Moore resonance evaluation in the energy range 0 to 2250 eV;**

- **Total of 3193 resonances including the external levels;**

- **Five parameters:**
  - **Resonance energy E_r**
  - **Gamma width Γ_γ,**
  - **Neutron width Γ_n**
  - **Two fission widths Γ_{f1} and Γ_{f2}**
  - **Total of 15965 parameters;**

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Covariance Evaluations for ^{235}U

- **"Retroactive" based on real experimental data**

- **Resonance Parameter Covariance Matrix (RPCM) generated**
  - **LCOMP=1 option**
  - **RPCM size of 1.76 Gigabytes (FILE32)**

- **Conversion from FILE32 into FILE33, i.e., Cross Section Covariance Matrix (CSCM)**
  - **522 energy boundaries used**
  - **CSCM size of 30 megabytes**

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Covariance Evaluations for ^{238}U

- **Reich-Moore resonance evaluation in the energy range 0 to 20 keV;**

- **Total of 3343 resonances including the external levels;**

- **Five parameters:**
  - **Resonance energy E_r**
  - **Gamma width Γ_γ,**
  - **Neutron width Γ_n**
  - **Total of 10029 parameters;**

paradigm shift

Covariance Evaluations for ^{238}U

- **"Retroactive" based on real experimental data**

- **Resonance Parameter Covariance Matrix (RPCM) generated**
  - **LCOMP=1 option**
  - **RPCM size of 800 megabytes (FILE32)**

- **Conversion from FILE32 into FILE33, i.e., Cross Section Covariance Matrix (CSCM)**
  - **535 energy boundaries used**
  - **CSCM size of 200 kilobytes**

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Covariance Evaluations for ^{239}Pu

- **Reich-Moore resonance evaluation in the energy range 0 to 2500 keV;**

- **Total of 1030 resonances including the external levels;**

- **Five parameters:**
  - **Resonance energy E_r**
  - **Gamma width Γ_γ,**
  - **Neutron width Γ_n**
  - **Two fission widths Γ_{f1} and Γ_{f2}**
  - **Total of 5150 parameters;**

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Covariance Evaluations for ^{239}Pu

- **Retroactive based on real experimental data and data generated from resonance parameter**

- **Resonance Parameter Covariance Matrix (RPCM) generated**
  - LCOMP=1 option
  - RPCM size of **2.5 megabytes** (FILE32)

- **Conversion from FILE32 into FILE33, i.e., Cross Section Covariance Matrix (CSCM)**
  - 535 energy boundaries used
  - CSCM size of **140 kilobytes**

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SUMMARY

Isotope	LCOMP=1	
	RPCM	CSCM
^{233}U	100 megabytes	3 megabytes
^{235}U	1.76 gigabytes	30 megabytes
^{238}U	800 megabytes	200 kilobytes
^{239}Pu	2.5 megabytes	140 kilobytes

Detail information can be found at:

Nuclear Data Sheets

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