UT-BATTELLE

Nuclear Data Covariance Generation in the Resonance Region

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CSEWG & USNDP Meetings

Brookhaven National Laboratory

November 8 - 11, 2005

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

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).**

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

  Covariance generated from existing resonance evaluation

Current status of ENDF covariances

- **Some of the ENDF/VI evaluations do not have covariances for resonance parameters.**
  - **These need to be inserted into the ENDF File 32 if they are not there already.**
- **What can be done if File 32 is empty?**
  - **“Best solution” = reanalyze, and generate File 32 along with File 2**
  - **“Best solution” is not practical on a reasonable time scale. We want to keep the File 2 parameters and simply add File 32 covariances.**

ENDF File 32 (parameter covariance matrix)

- **Needed: a method for retroactively generating the covariance matrix and writing it into File32 format**

- **SAMMY has such a scheme**

Retroactive covariance scheme

1. **Pick representative data sets covering the energy range of the R-matrix evaluation**
2. **Do simultaneous fit to all those data sets**
   - **Take ENDF File 2 Parameters for initial values**
   - **Flag all resonance parameters**
     - **so that they are treated as variables in the fitting procedure**

Retroactive covariance scheme, cont.

3. **Check whether output parameter values are very different from input**
   - **Hopefully there are not significant changes**
4. **Assume that the output parameter covariance matrix is a reasonable approximation to use in conjunction with the original (input) parameter values**
5. **Write the output parameter covariance matrix into File 32 format**

Details, cont.

1. Do simultaneous fit to all those data sets

- **Start from Bayes' Equations (generalized least-squares)**

$$P' = P + M' Y \qquad M' = (M^{-1} + W)^{-1}$$

$$Y = G^{t} V^{-1} (D - T) \qquad W = G^{t} V^{-1} G$$

Notation: (primes indicate updated values)

P = parameters
M = covariance matrix for parameters
D = experimental data
T = theoretical calculation
G = partial derivatives (sensitivity matrix)
V = covariance matrix for experimental data

Details, cont.

- **Bayes' Equations** in a slightly different form

$$P' = P + M' Y \qquad \text{where } Y = \Sigma_i Y_i$$

$$\text{with } Y_i = G_i^t V_i^{-1} (D_i - T_i) \qquad \text{for data set } i$$

$$M' = (M^{-1} + W)^{-1} \qquad \text{where } W = \Sigma_i W_i$$

$$\text{with } W_i = (G_i^t V_i^{-1} G_i) \qquad \text{for data set } i$$

- **Treat individual data sets separately, calculating Y_i and W_i using ENDF values for resonance parameters**
- **Add Y_i's and W_i's to obtain Y and W**
- **Solve Bayes' equations once to fit all data sets**

Details, cont.

2. **Check whether output parameter values = input values**

   Question: **Is it true that** $P' \approx P$ **?**

   Answer: **Probably, because** $Y = G^t V^{-1} (D - T) \approx 0$

   because D **was chosen** $\approx T$

3. **Assume** M' **is appropriate for** P

4. **Write** M' **in ENDF File32 format**

Covariance Processing Tools

- **NJOY**
  - **Not capable of processing RM covariance data**
- **PUFF**
  - **ORNL capability for covariance processing. Recently modified to accommodate new R-matrix resonance formats and to perform accurate calculations of covariance matrices for multigroup cross sections (Doro Wiarda).**
- **ERRORJ**
  - **Process most of R-matrix covariance data**

Application

^{233}U Covariance Matrix

A full ^{233}U resonance covariance matrix has been computed

- **SAMMY array size determined as**
  - **No. of resonances**
  - **No. of varied parameters per resonance**
  - **No. of data points**
- **For ^{233}U:**
  - **No. of resonances = 769**
  - **No. of varied parameters per resonance = 5**
  - **No. of data points = 20,000**
  - **SAMMY array size = 76,900,000**
- **Memory = 76,900,000 * 8 bytes**

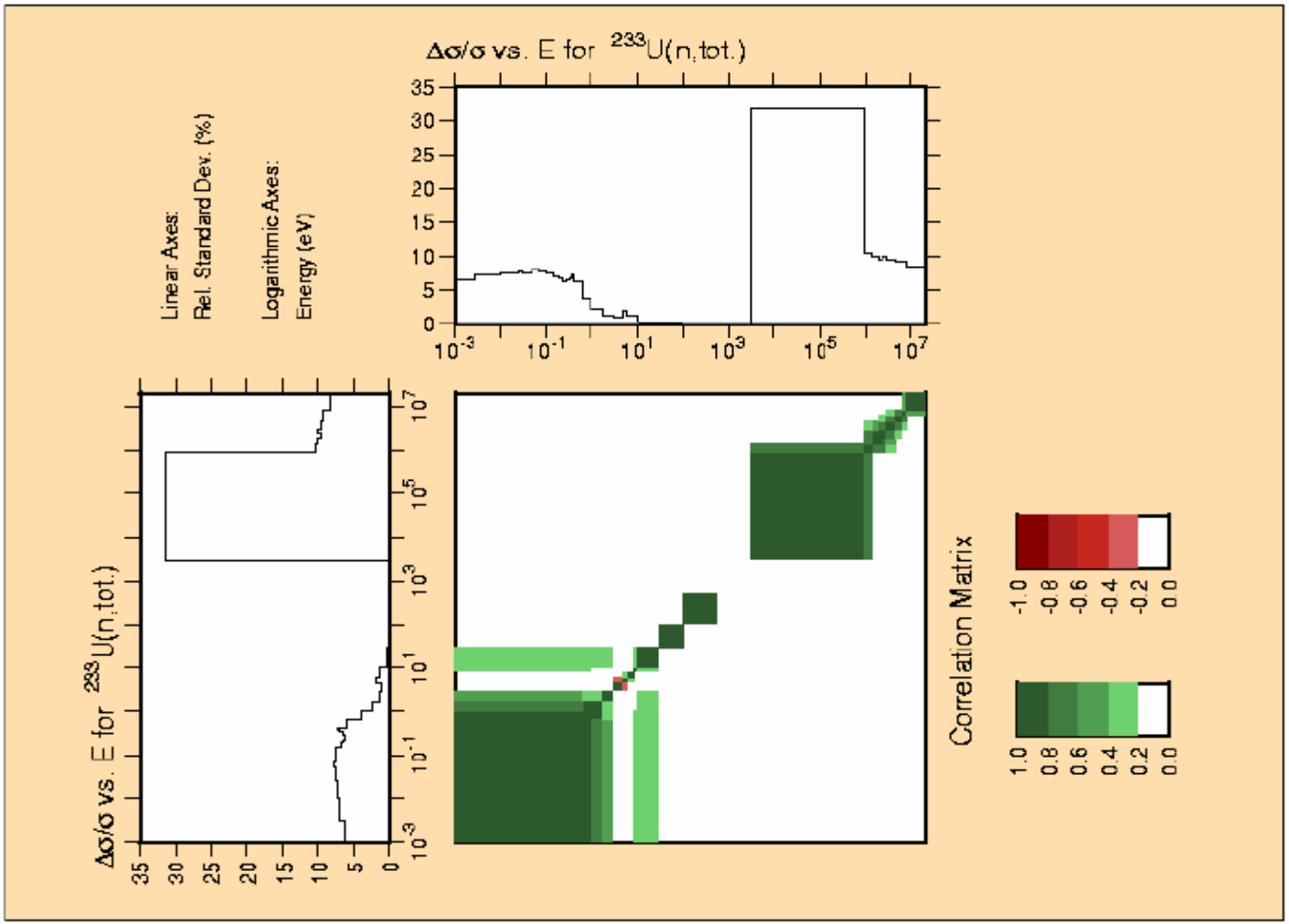
  ~ 700 MB
- **In-house ORNL computers (32 gigabytes memory) able to handle this requirements !!**

Compact Format

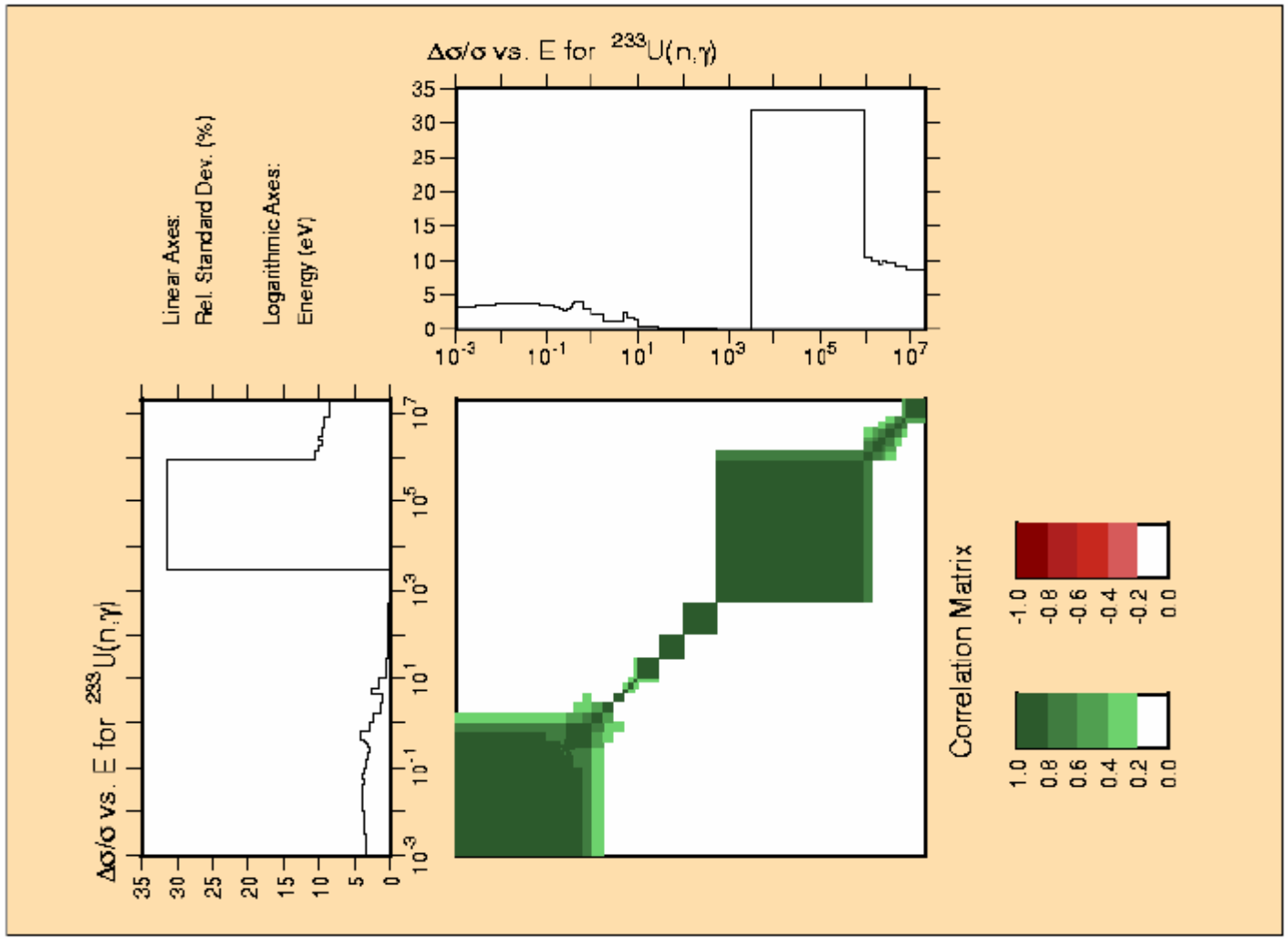
WHY IS IT NEEDED ?

- **100 megabytes of storage would be required to represent the ^{233}U covariance using existing ENDF format**
- **Compact format needs only 2 megabytes for representing ^{233}U covariance data**
- **In the compact formalism correlation coefficients (-1.0 and +1.0) are mapped into signed integer numbers from -99 to 99 and correlations less than 2 % are dropped**
- **Further reduction of storage can be achieved by dropping correlations less than an arbitrary value**

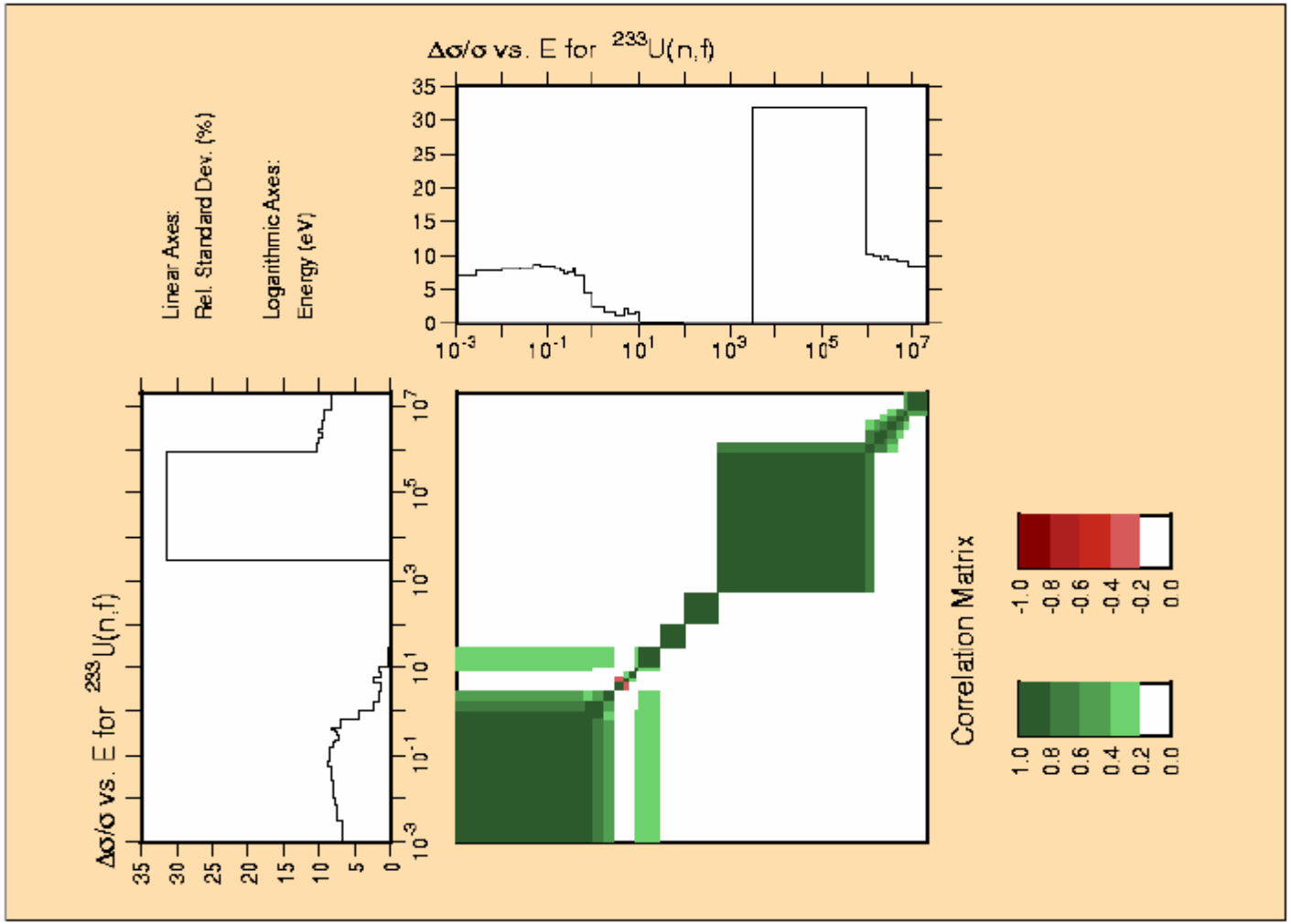
ERRORJ Processed Covariance (Total Cross Section)



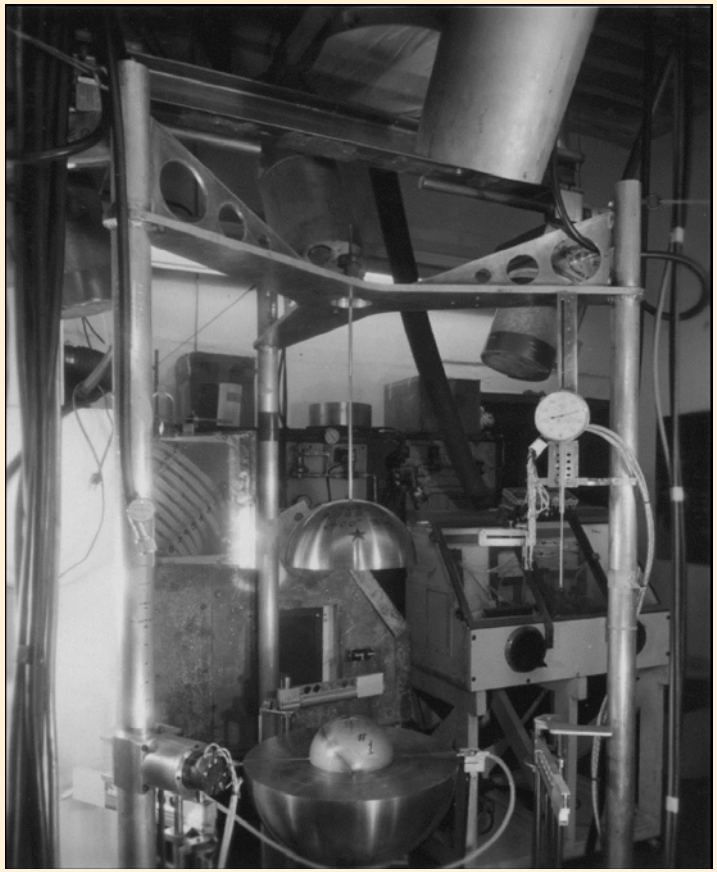
ERRORJ Processed Covariance (Capture Cross Section)



ERRORJ Processed Covariance (Fission Cross Section)

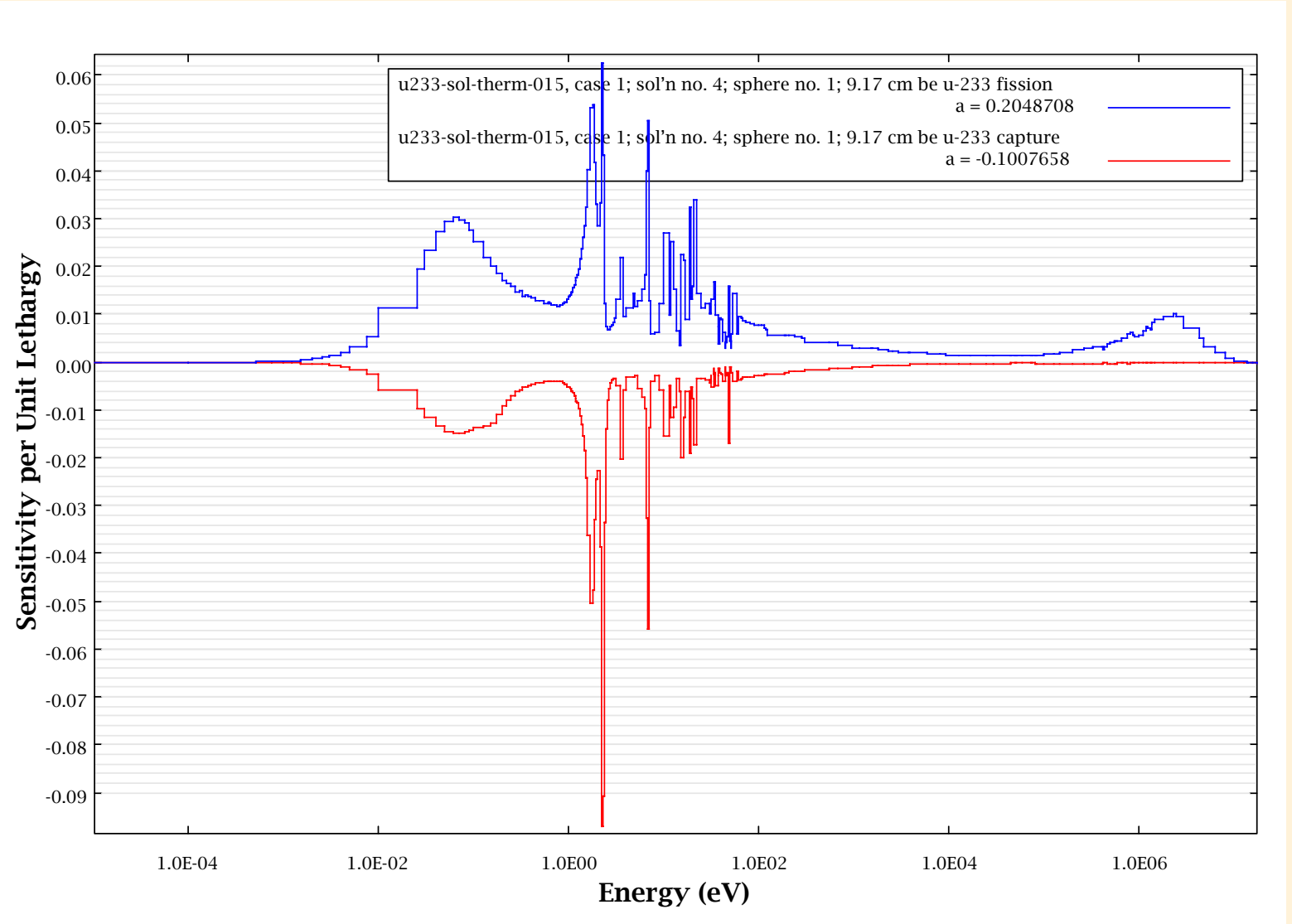


Overview of Experiment (u233-sol-therm-015)



A series of criticality studies were performed at Lawrence Livermore National Laboratory in the late 1950's using aqueous solutions of ^{233}U in the form of UO_2F_2 stabilized with 0.3% by weight of HF.

Sensitivity to the capture and fission cross section for the u233-sol-therm-015 benchmark



Results from u233-sol-therm-015 benchmark (case 1)

Forward Calculation k_{eff} : 0.99470367

Adjoint Calculation k_{eff} : 0.99451532

^{233}U contribution to standard deviation of k_{eff} : 0.5112%

^{233}U Contributions *10^4 by reaction pairs to relative covariance of k_{eff}

	fission	n, gamma	elastic
fission	**3.9622E-01**	**-1.0552E-01**	**-2.4250E-06**
n, gamma	**-1.0552E-01**	**7.9620E-02**	**9.8695E-07**
elastic	**-2.4250E-06**	**9.8695E-07**	**3.0737E-08**

Concluding Remarks

- **Cross section and covariance evaluation in the resonance region were done for ^{233}U**
- **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;**
- **Benchmark calculations were done with the TSUNAMI code;**
- **Procedure will be used for other Isotope;**