# Resonance Region Covariance Analysis Method and New Covariance Data for $^{232}Th$, $^{233}U$, $^{235}U$, $^{238}U$, and $^{239}Pu$

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# OUTLINE

- Resonance Region Covariance Evaluations at ORNL for $^{233}U$, $^{235}U$, $^{238}U$, $^{239}Pu$, and $^{232}Th$;
- Compact formalism;
- FILE32 to FILE33 conversion;
- Applications: $^{238}U$ data uncertainty propagation in $k_{eff}$ calculations;
- Concluding remarks;

# Available Covariance Data in ENDF

## Contents of File Types (MF)

MF=30: sensitivity data covariance files

MF=31: covariances for average number of neutrons per fissions

MF=32: covariances for resonance parameters

MF=33: covariances for reaction cross sections

MF=34: covariances for angular distributions

MF=35: covariances for energy distributions

MF=36: covariances for angle-energy distributions

MF=37~38: null

MF=39: covariances for radionuclide production yields

MF=40: covariances for radionuclide production cross sections

# Covariance Evaluations

**a) Resonance covariance evaluations have been done for $^{233}$U, $^{235}$U, $^{238}$U, $^{239}$Pu, and $^{232}$Th**

**b) LCOMP=1 format used; LCOMP=2 (compact formalism used); Conversion FILE32 to FILE33 done**

**c) High energy covariance provided by LANL for $^{233}$U, $^{235}$U, $^{238}$U and $^{239}$Pu were merged with ORNL resonance evaluations; IAEA also provided covariance data for $^{233}$U in the high energy region;**

**d) Evaluation for $^{232}$Th done under IAEA/CRP**

**e) New cross section and covariance evaluation for $^{239}$Pu**

# Covariance Evaluation Procedure

**SAMMY Code:**

**a)** Retroactive covariance: Obtained when no experimental data exist (use experimental data whenever possible). Otherwise, use educated guess on "pseudo" experimental data generation;

**b)** Direct generation of covariance: Done in the flow of the evaluation;

**SAMMY format to ENDF format**

SAMMY generated resonance covariance can be converted into the ENDF format (FILE 32 SECTION 2151)

LCOMP=1 ➡ Entire covariance data explicitly given

LCOMP=2 ➡ Compact format

# Covariance Generated with LCOMP=1

| Isotope | Lcomp=1<br><br>FILE32 |
|---|---|
| $^{232}$Th | 55 MB |
| $^{233}$U | 100 MB |
| $^{235}$U | 1.8 GB |
| $^{238}$U | 700 MB |
| $^{239}$Pu | 190 MB |

# Compact Formalism

Covariance matrix element connecting parameter number $i$ with parameter number $j$ is denoted by $V_{ij}$, the uncertainty on parameter $i$ by $D_i$, and the correlation coefficient by $C_{ij}$, then these quantities are related by

$$D_i^2 = V_{ii} \qquad V_{ij} = D_i C_{ij} D_j$$

Values for $C_{ij}$ range from −1 to +1; values for $D_i$ are always positive. Note that the diagonal elements of $C_{ij}$, those for which $i = j$, are always exactly 1.0 and therefore are never specified explicitly. Compacting the off-diagonal correlation coefficients is accomplished as follows:

1. Drop (set to zero) all values of $C_{ij}$ between $-10^{-\text{NDIGIT}}$ and $+10^{-\text{NDIGIT}}$. (NDIGIT are 2 through 6)

2. Multiply the remaining coefficients by $10^{\text{NDIGIT}}$.

3. Map all positive values greater than K and less than or equal to K+1 to the integer K.

4. Map all negative values less than −K and greater than or equal to −K−1 to the integer −K.

# Conversion from FILE32 to FILE33

## Averaged Group Cross Sections

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

**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***

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

**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 the resonance parameter covariance stored in the ENDF library (FILE32)**

# 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.**

# Question:
# Can one find an equivalence ?

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

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

# 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(σ)* such that the uncertainty in the group cross section reproduces that using the FILE32 representation;**

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

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

# Energy Mesh Used

| Isotope | Energy Range (eV) | Energy Mesh |
|---|---|---|
| $^{232}$Th | $10^{-5}$ - 4000 | - |
| $^{233}$U | $10^{-5}$ – 600 | 329 |
| $^{235}$U | $10^{-5}$ – 2250 | 522 |
| $^{238}$U | $10^{-5}$ – 20000 | 535 |
| $^{239}$Pu | $10^{-5}$ – 2500 | 318 |

# Size Reduction Estimation

| Isotope | Lcomp=1<br>FILE32 | FILE33 | Lcomp=2<br>File32<br>(compact) |
|---|---|---|---|
| $^{232}$Th | 55 MB | - | 320 KB |
| $^{233}$U | 100 MB | 12 MB | - |
| $^{235}$U | 1.8 GB | 30 MB | - |
| $^{238}$U | 700 MB | 33 MB | 16 MB |
| $^{239}$Pu | 190 MB | 11 MB | - |

# ORNL TOOS FOR CROSS SECTION AND COVARIANCE GENERATION AND PROCESSING

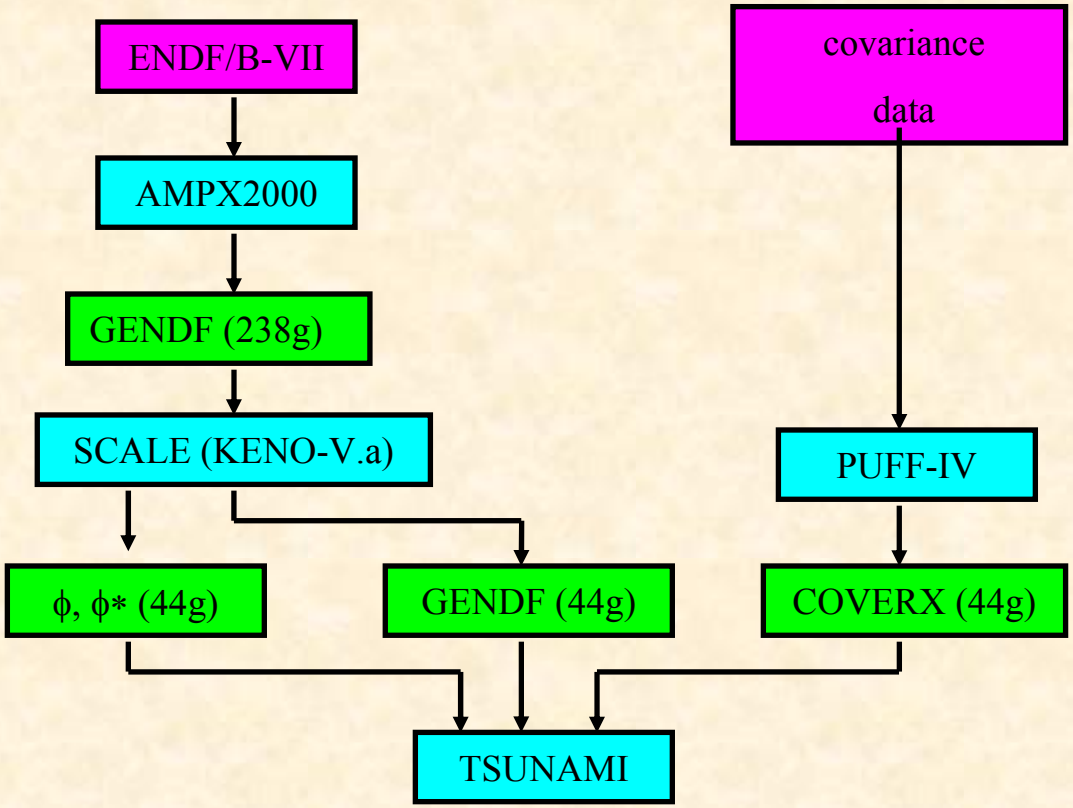
- Cross section evaluation done with the SAMMY code
- Data processing done with the AMPX code
- Uncertainty data processing done with the PUFF-IV code

Sensitivity Analysis
done with the TSUNAMI Code

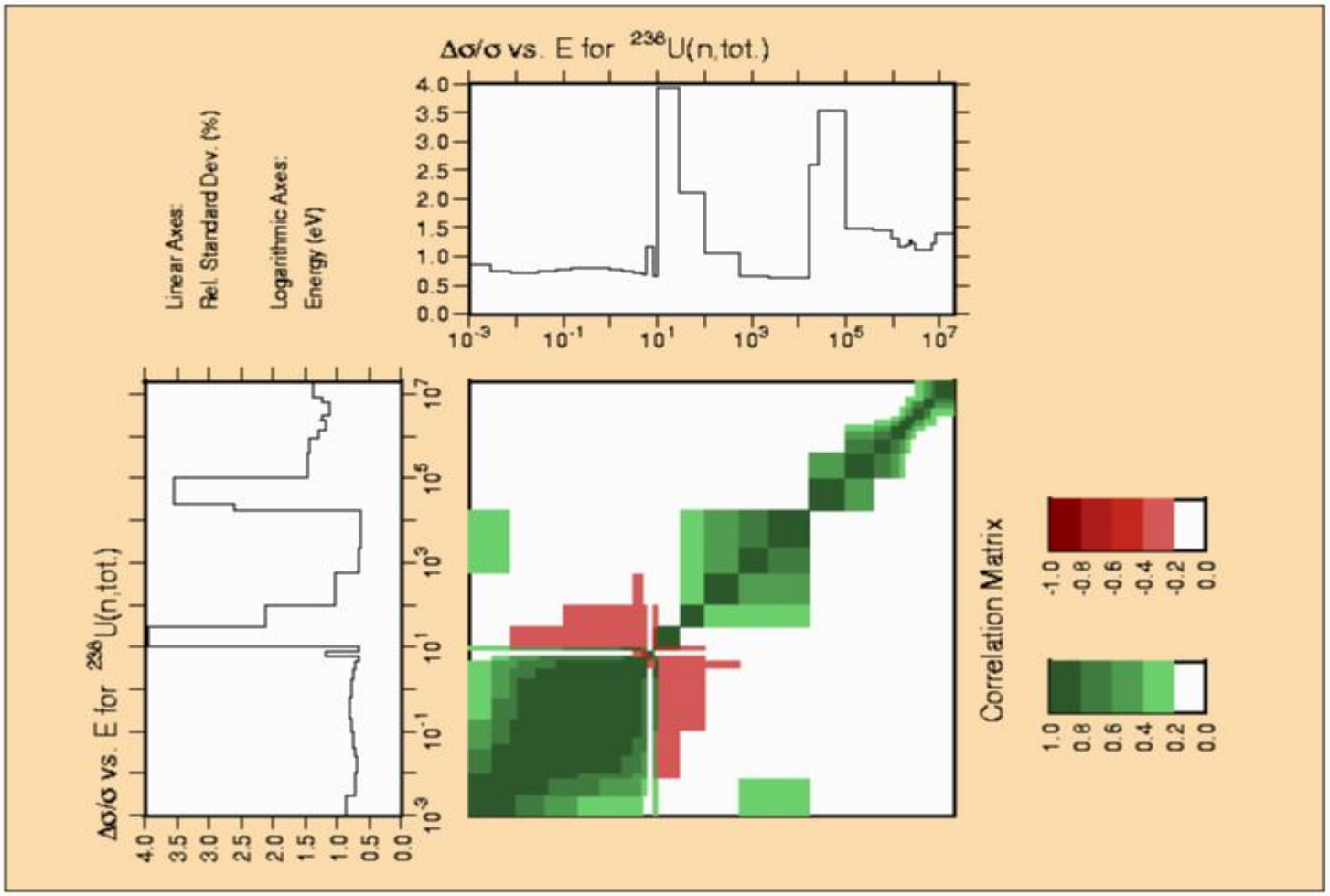
# Application

- Covariance data generated with the PUFF-IV code in the COVERX format were used in benchmark calculations with the code TSUNAMI for $^{238}U$
- The calculations were done with the SCALE 238-group ENDF/B-V cross-section data library, for which the $^{238}U$ evaluation in the SCALE library was replaced by the new $^{238}U$ ENDF/B-VII cross-section evaluation
- The AMPX code was used to process the cross sections in the 238-group structure.
- Uncertainty in the multiplication factor $k_{eff}$ was investigated is the LEU-SOL-THERM-001 (SHEBA-II)

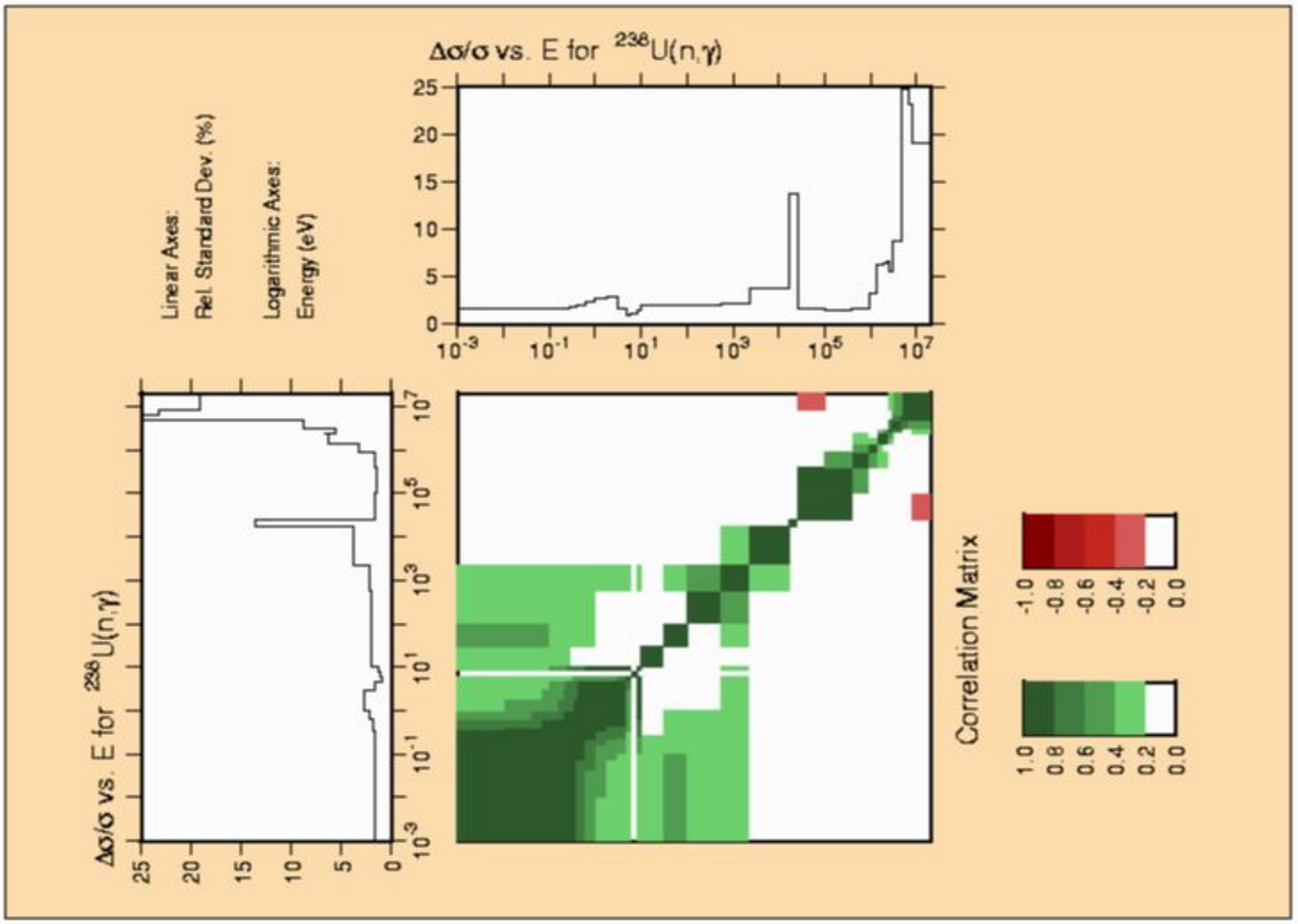
# Data flow for sensitivity and uncertainty calculation with TSUNAMI



# Total cross section covariance (processed with PUFF-IV )



# Capture cross section covariance (processed with PUFF-IV )



# Group-averaged capture cross section in the 44-group structure

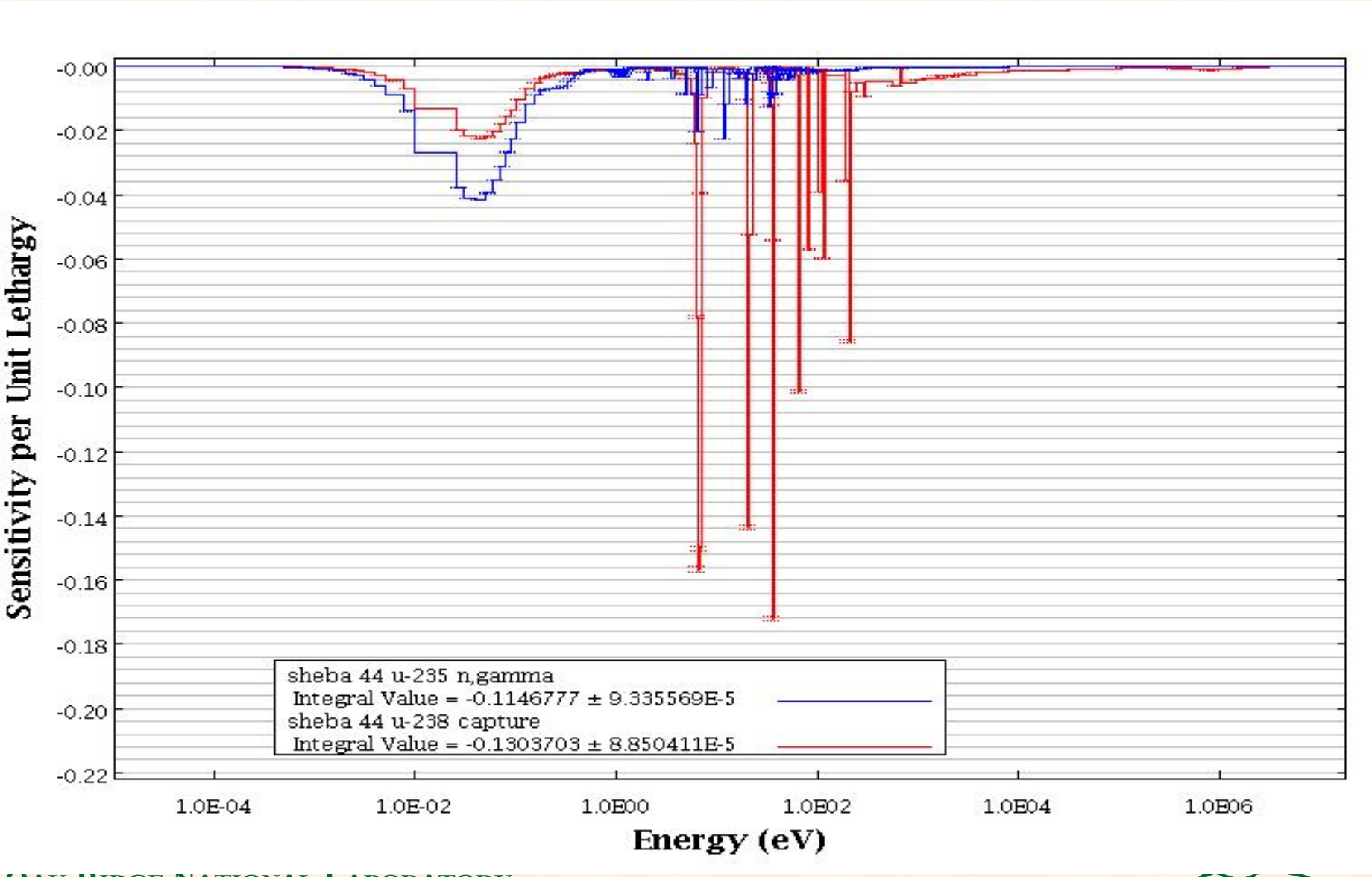
| Group | Energy Range (eV) | Cross Section (b) | Rel.s.d | Std.dev |
|---|---|---|---|---|
| 28 | 0.37500–0.35000 | 0.748110 | 0.020130 | 0.015059 |
| 29 | 0.35000–0.32500 | 0.772380 | 0.019840 | 0.015324 |
| 30 | 0.32500–0.27500 | 0.815530 | 0.019434 | 0.015849 |
| 31 | 0.27500–0.25000 | 0.864830 | 0.019104 | 0.016522 |
| 32 | 0.25000–0.22500 | 0.905830 | 0.018894 | 0.017115 |
| 33 | 0.22500–0.20000 | 0.954110 | 0.018712 | 0.017853 |
| 34 | 0.20000–0.15000 | 1.050100 | 0.018491 | 0.019417 |
| 35 | 0.15000–0.10000 | 1.253900 | 0.018307 | 0.022954 |
| 36 | 0.10000–0.07000 | 1.501500 | 0.018302 | 0.027480 |
| 37 | 0.07000–0.05000 | 1.770600 | 0.018333 | 0.032461 |
| 38 | 0.05000–0.04000 | 2.025100 | 0.018390 | 0.037241 |
| 39 | 0.04000–0.03000 | 2.295300 | 0.018424 | 0.042288 |
| 40 | 0.03000–0.02530 | 2.573600 | 0.018448 | 0.047478 |
| 41 | 0.02530–0.01000 | 3.257000 | 0.018509 | 0.060285 |
| 42 | 0.01000–0.00750 | 4.555800 | 0.018570 | 0.084601 |
| 43 | 0.00750–0.00300 | 5.869300 | 0.018585 | 0.109080 |
| 44 | 0.00300–0.00001 | 10.44500 | 0.018612 | 0.194400 |

# Group-averaged capture cross section in the 44-group structure

| Group | Energy Range (eV) | Cross Section (b) | Rel.s.d | Std.dev |
|---|---|---|---|---|
| 13 | 20000.000–17000.000 | 0.517430 | 0.144000 | 0.074509 |
| 14 | 17000.000–3000.0000 | 0.812190 | 0.044108 | 0.035824 |
| 15 | 3000.0000–550.00000 | 2.278900 | 0.022072 | 0.050300 |
| 16 | 550.00000–100.00000 | 11.205000 | 0.021179 | 0.237300 |
| 17 | 100.00000–30.00000 | 45.044998 | 0.023170 | 1.043700 |
| 18 | 30.00000–10.00000 | 60.556999 | 0.019940 | 1.207500 |
| 19 | 10.00000–8.10000 | 0.783020 | 0.015348 | 0.012018 |
| 20 | 8.10000–6.00000 | 424.470001 | 0.011897 | 5.050100 |
| 21 | 6.00000–4.75000 | 2.874800 | 0.010169 | 0.029232 |
| 22 | 4.75000–3.00000 | 0.779960 | 0.019184 | 0.014963 |
| 23 | 3.00000–1.77000 | 0.471900 | 0.031793 | 0.015003 |
| 24 | 1.77000–1.00000 | 0.474280 | 0.030767 | 0.014592 |
| 25 | 1.00000–0.62500 | 0.548210 | 0.025677 | 0.014076 |
| 26 | 0.62500–0.40000 | 0.654120 | 0.021826 | 0.014277 |
| 27 | 0.40000–0.37500 | 0.726340 | 0.020433 | 0.014841 |
| 28 | 0.37500–0.35000 | 0.748110 | 0.020130 | 0.015059 |

# APPLICATION: LEU-SOL-THERM-001
## (unreflected assembly, fueled with aqueous solution of approximately 5% enriched uranyl fluoride)

# Sensitivity of the multiplication factor to the capture cross section of $^{238}U$ and capture cross section of $^{235}U$



# Contribution to uncertainty in $k_{eff}$ by individual components or cross-correlations of the various $^{238}$U cross sections, in units of % $\Delta k/k$

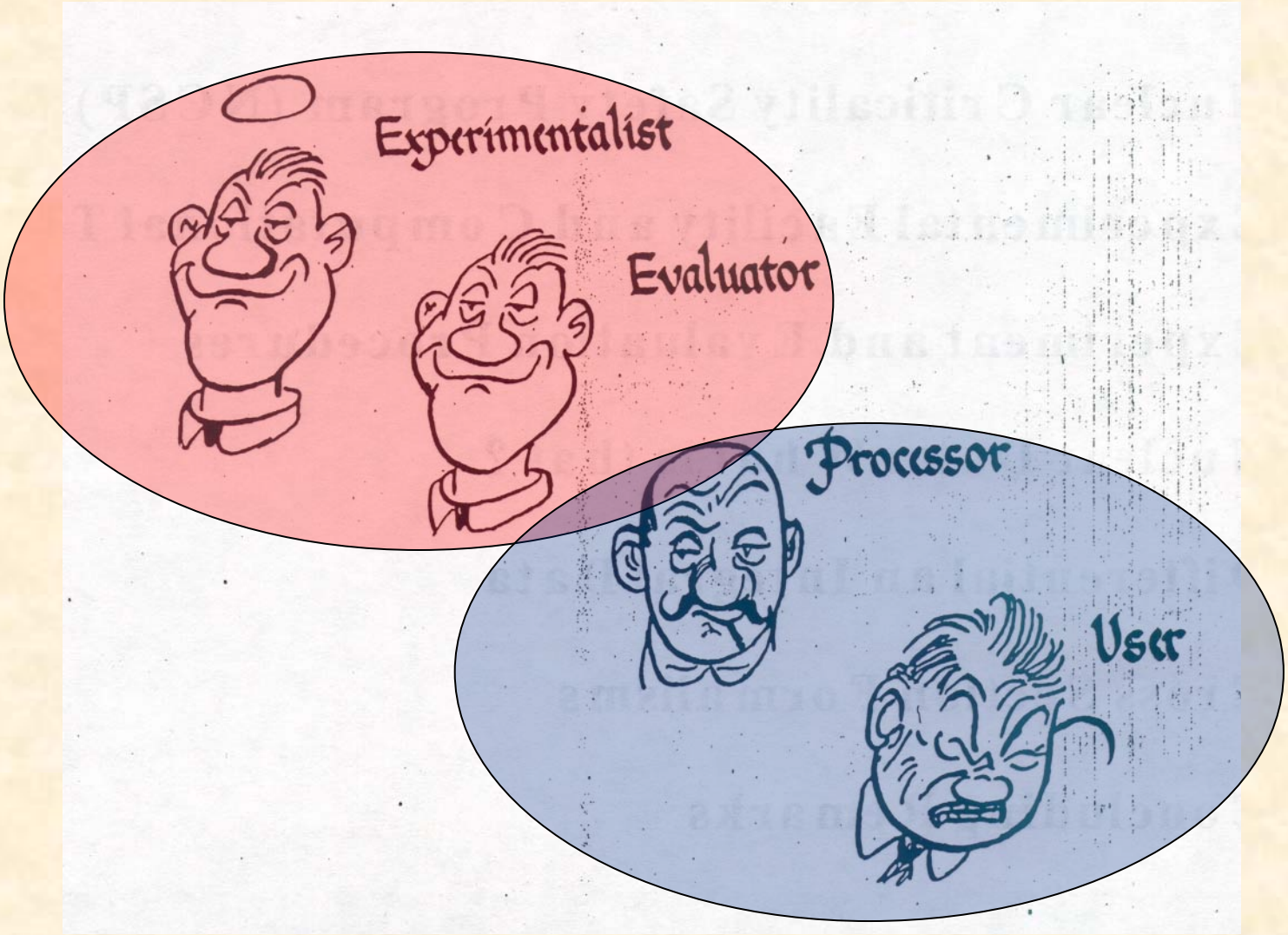
| | n,n' | n,gamma | elastic | nubar | n,2n | fission |
|---|---|---|---|---|---|---|
| n,n' | 0.15102 ± 0.00008 | | | | | |
| n,gamma | | 0.14788 ± 0.000005 | | | | |
| elastic | − 0.073720 ± 0.000044 | 0.0049657 ± 0.0000231 | 0.033494 ± 0.000020 | | | |
| nubar | | | | 0.020799 ± .000001 | | |
| n,2n | | | − 0.00080726 ± 0.00000032 | | 0.0072928 ± .0000032 | |
| fission | | 0.00052855 ± 0.00000002 | − 0.00085442 ± 0.00078239 | | | 0.0064727 ± .0000004 |

# RESUTS

- Calculations with TSUNAMI using the $^{238}$U ENDF/B-V 238-group cross section give $k_{eff}$ = 1.008398 ± 0.000296. (The quoted uncertainty is due to the stochastic aspect of the Monte Carlo calculation)
- Replacing the $^{238}$U ENDF/B-V cross section with the ENDF/B-VII cross section and keeping everything else the same produced a value for $k_{eff}$ of 1.004371 ± 0.000314
- The TSUNAMI-calculated percentage uncertainty in $k_{eff}$ due to the $^{238}$U data is 0.202191 ± 0.00001
- The percentage uncertainty of 0.202191 ± 0.00001 is obtained by squaring each individual correlation and adding (correlated data) or subtracting (anticorrelated data)

# Concluding Remarks

- **Resonance covariance evaluations were done for $^{233}$U, $^{235}$U $^{238}$U, $^{239}$Pu, and $^{232}$Th using SAMMY**
- **Compact formalism was used for $^{232}$Th**
- **FILE32 to FILE33 conversion done for $^{233}$U, $^{235}$U $^{238}$U, $^{239}$Pu (Note: FILE32 available)**
- **Covariance data processed with PUFF-IV**
- **Benchmark calculations were done with the SCALE sensitivity sequence TSUNAMI**
- **Example: $^{238}$U data uncertainty propagated into the $k_{eff}$ calculations**


Experimentalist
Evaluator
Processor
User

# Question?