# Covariance Evaluation for U-235, U-238, and Pu-239

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# Introduction

## Covariance Needs for Major Actinides

- LANL/T-16 is responsible to ENDF/B-VII for the covariance evaluation in the fast range for major actinides
- The most important data for nuclear technology applications are the covariances for U-235, U-238, and Pu-239
- Potential users of these covariance data are :
  - Criticality safety, AFCI, Gen-IV, GNEP, homeland security,. . .

## Capabilities of Covariance Processing and Utilization

- Evaluated covariance data are stored in an ENDF-6 format file
- The data are processed with NJOY-ERRORJ to obtain a grouped cross section covariance
- The group covariance data are applied to many properties of nuclear systems, such as $k_{\mathrm{eff}}$, to estimate their uncertainties
- Need a sensitivity study, or Monte Carlo technique

# Covariance Evaluation in the Fast Region

## Evaluation based on GNASH calculations

- We employed a GNASH-KALMAN technique
- Experimental errors (statistical and systematics) are from EXFOR and literature.

## Standards Evaluation

- Covariance data of U-235 and U-238 were taken from the standards covariance data with appropriate energy boundary adjustments.
- Correlations between different nuclides (light elements) were not included

## Least-Squares Calculations with SOK and GLUCS

- were applied to evaluate $\nu_p$ covariances

## Other Resources

- Th-232 (IAEA), Gd, Ir, Y, Tc (BNL)

# KALMAN Method

## GNASH-KALMAN Code System

- The KALMAN calculation includes statistical and systematic errors in the experimental data
  - correlation from the systematic errors
- Constraint by a physical model employed
  - correlation from a model which is used for interpolation
- Sensitivities are calculated with the T-16 cluster — almost automated
- The best sets of GNASH (or ECIS) input parameters were already selected by PGY for the ENDF/B-VII evaluations
- The GNASH run for the sensitivity calculation is not exactly the same as for the ENDF/B-VII, fission cross sections, for example
- However, we can assume that the sensitivities of model parameters to the calculated cross sections are not so different

# What About Elastic ?

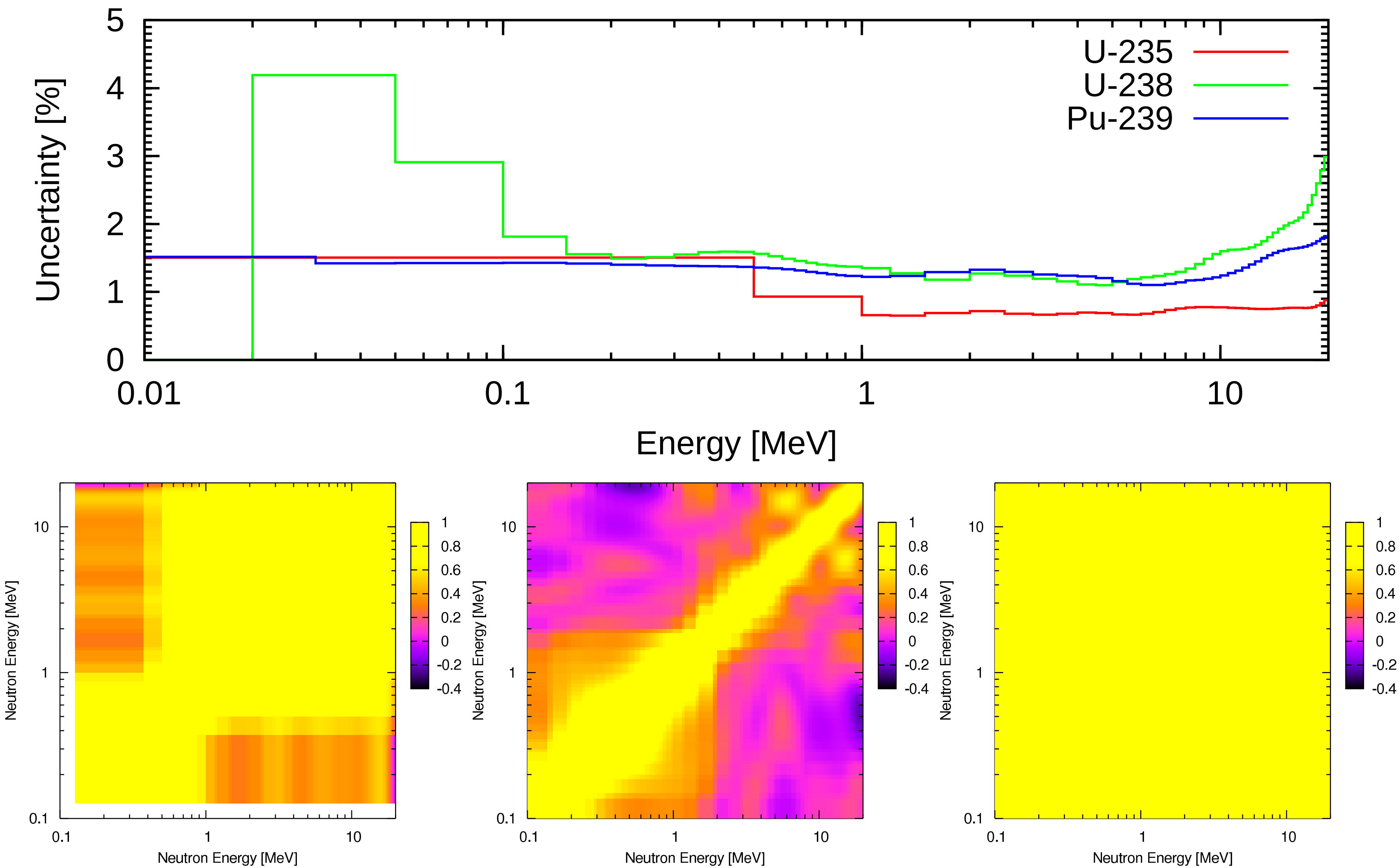
## LANL / BNL Evaluation

- Since the elastic cross sections are calculated by $\sigma_{tot} - \sum \sigma_i$, we simply give an elastic covariance in a similar way.
- Cov(elastic) = $\sum$ Cov(all other reactions), but correlations between them are $-1$

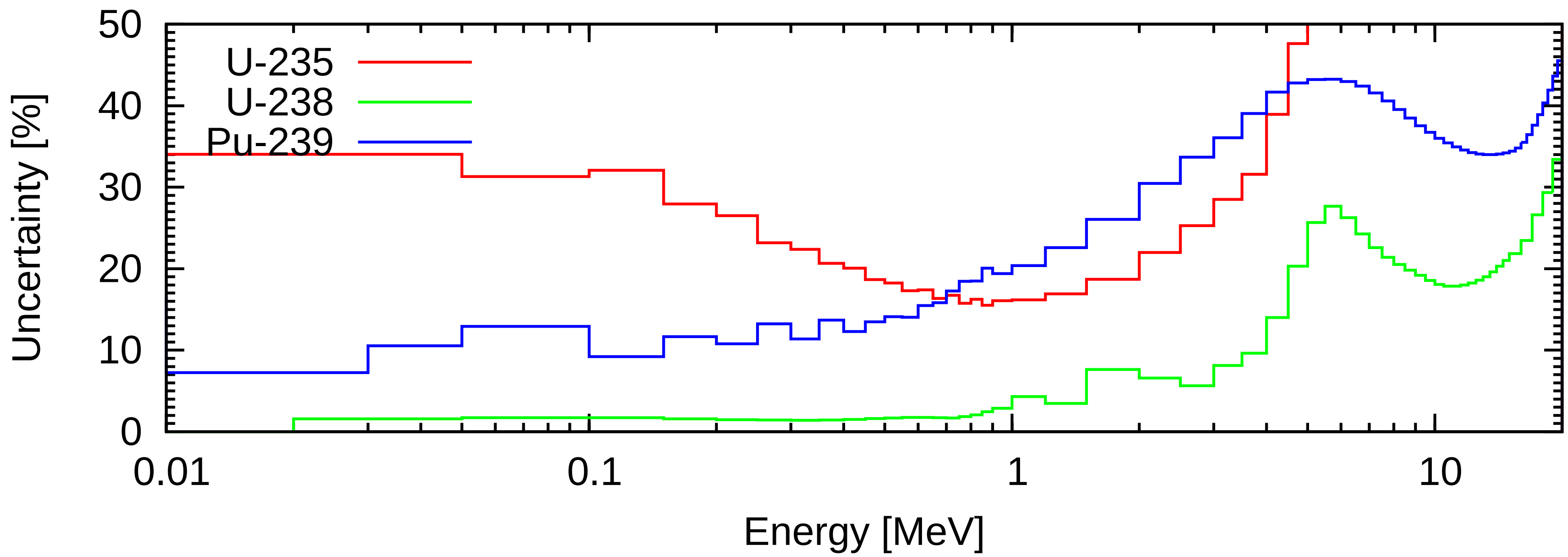
## IAEA Evaluation for Th-232

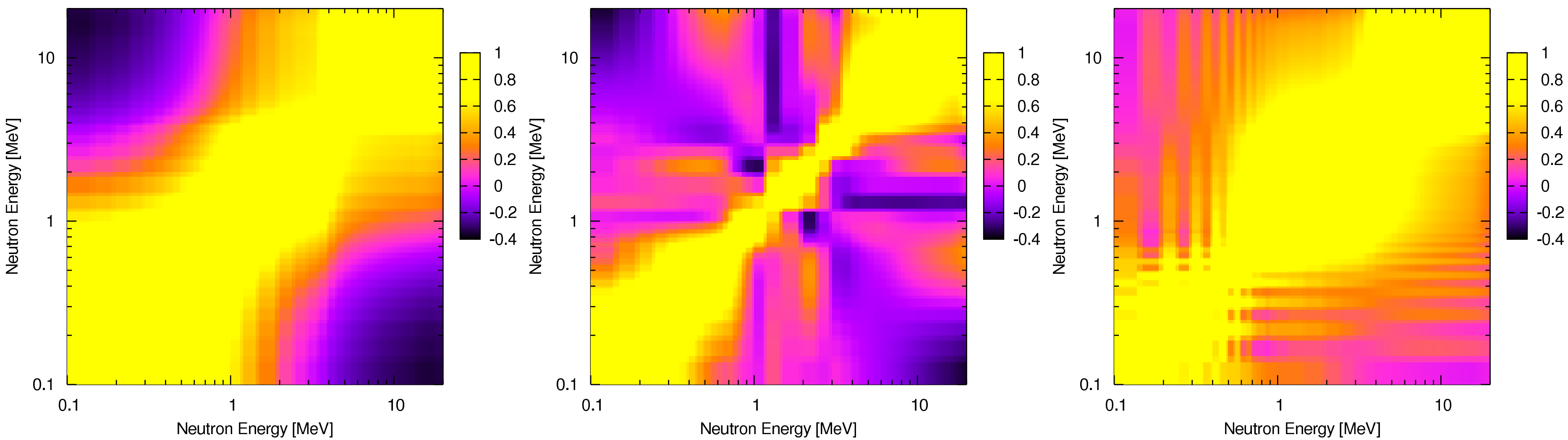
- Elastic covariance (MF33, MT2) is given
- MF3, MT1 is constructed from all partial cross sections
- MF33, MT5 is given

# Total Cross Section

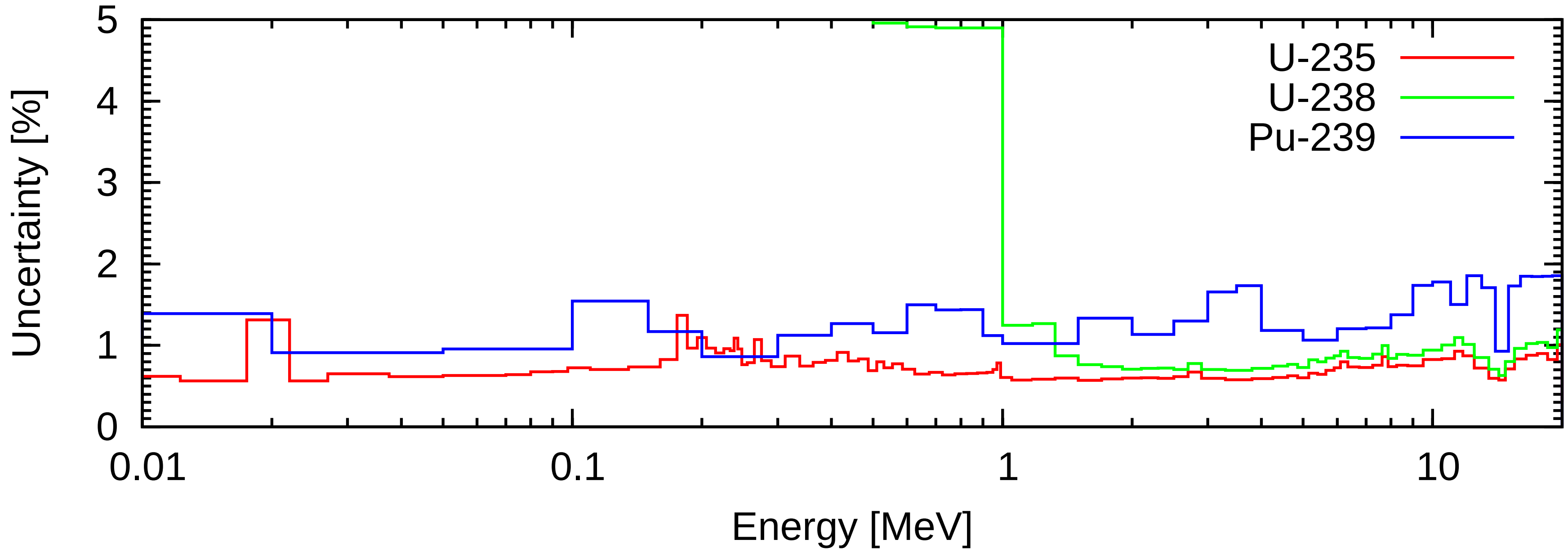


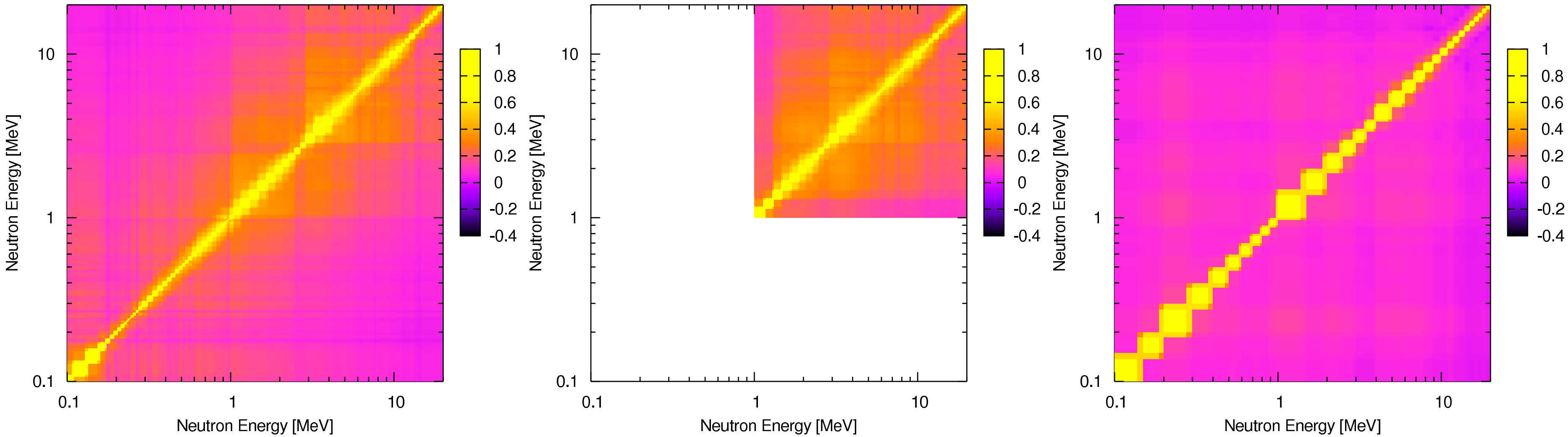
# Capture Cross Section



# Fission Cross Section

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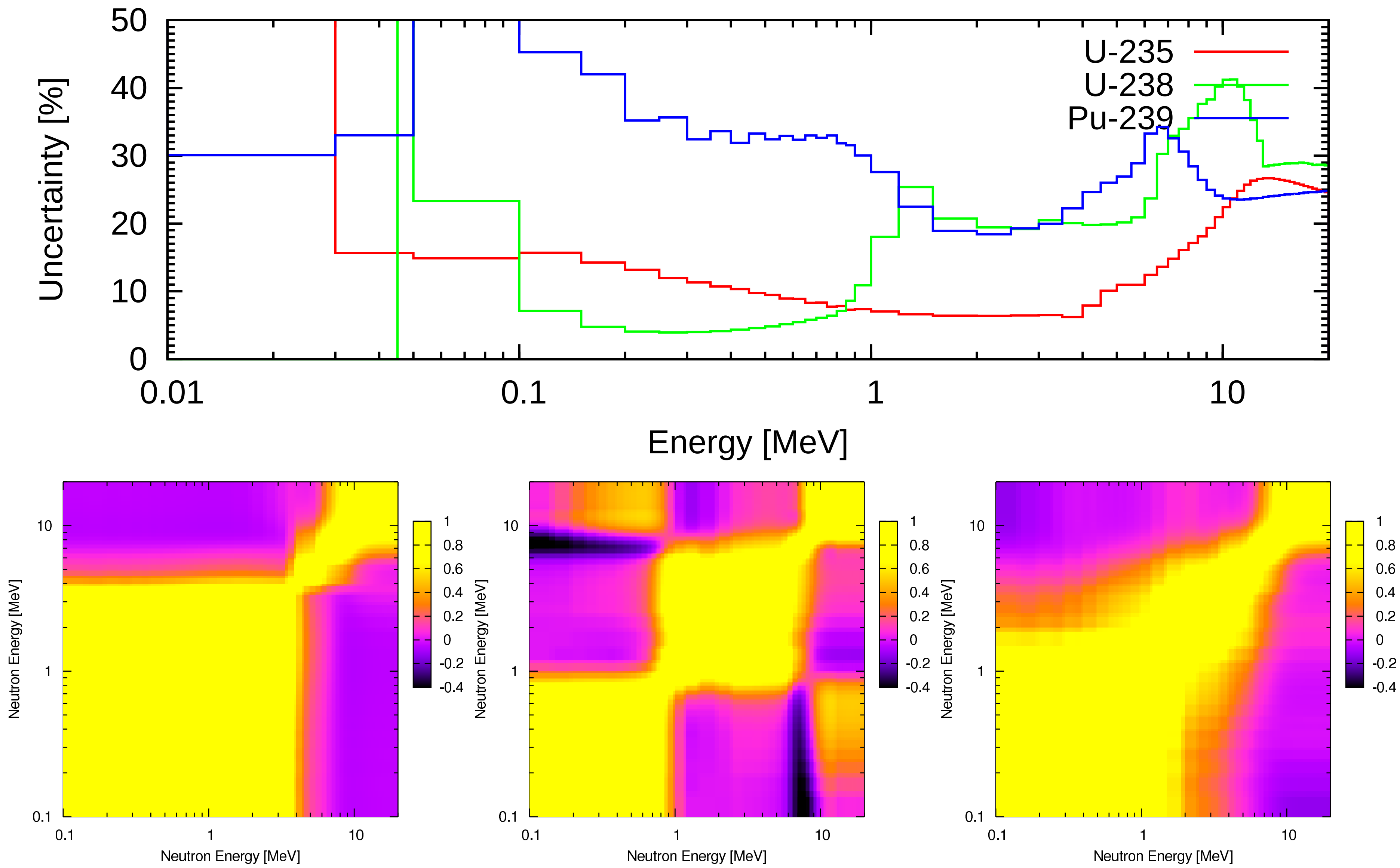
# Inelastic Cross Section

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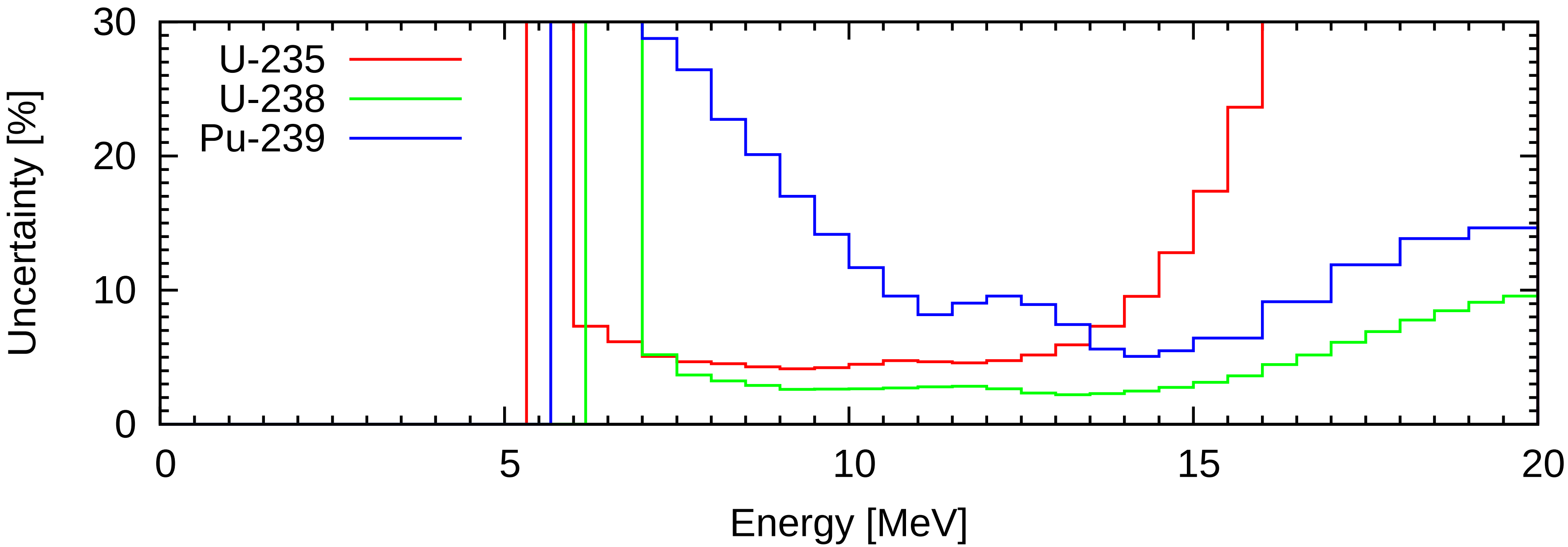
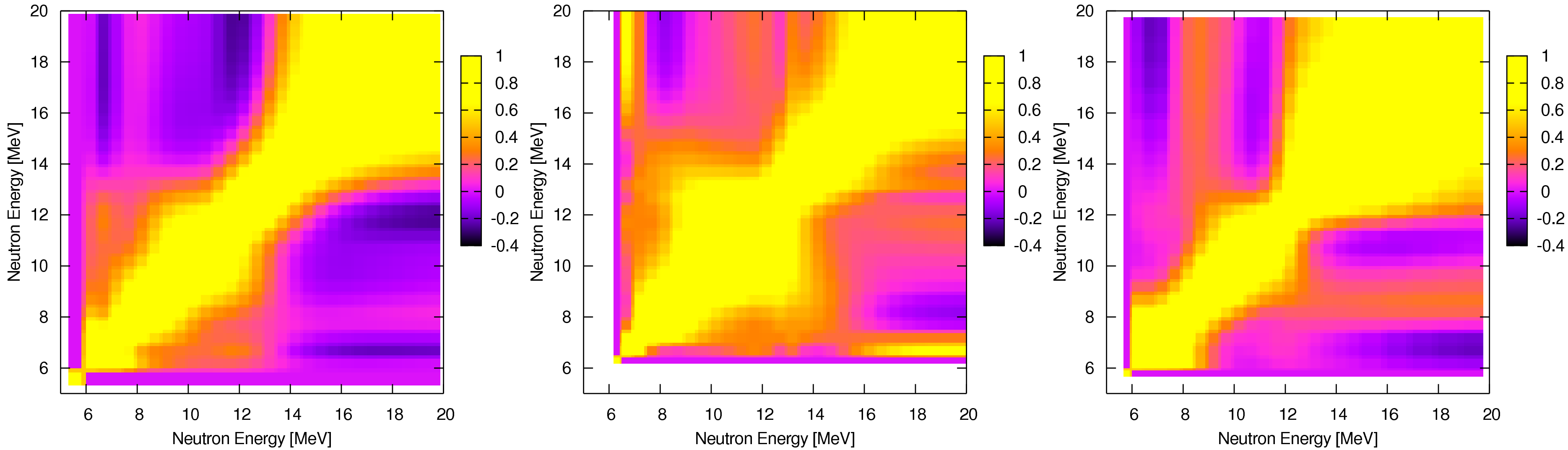
# (n,2n) Reaction Cross Section

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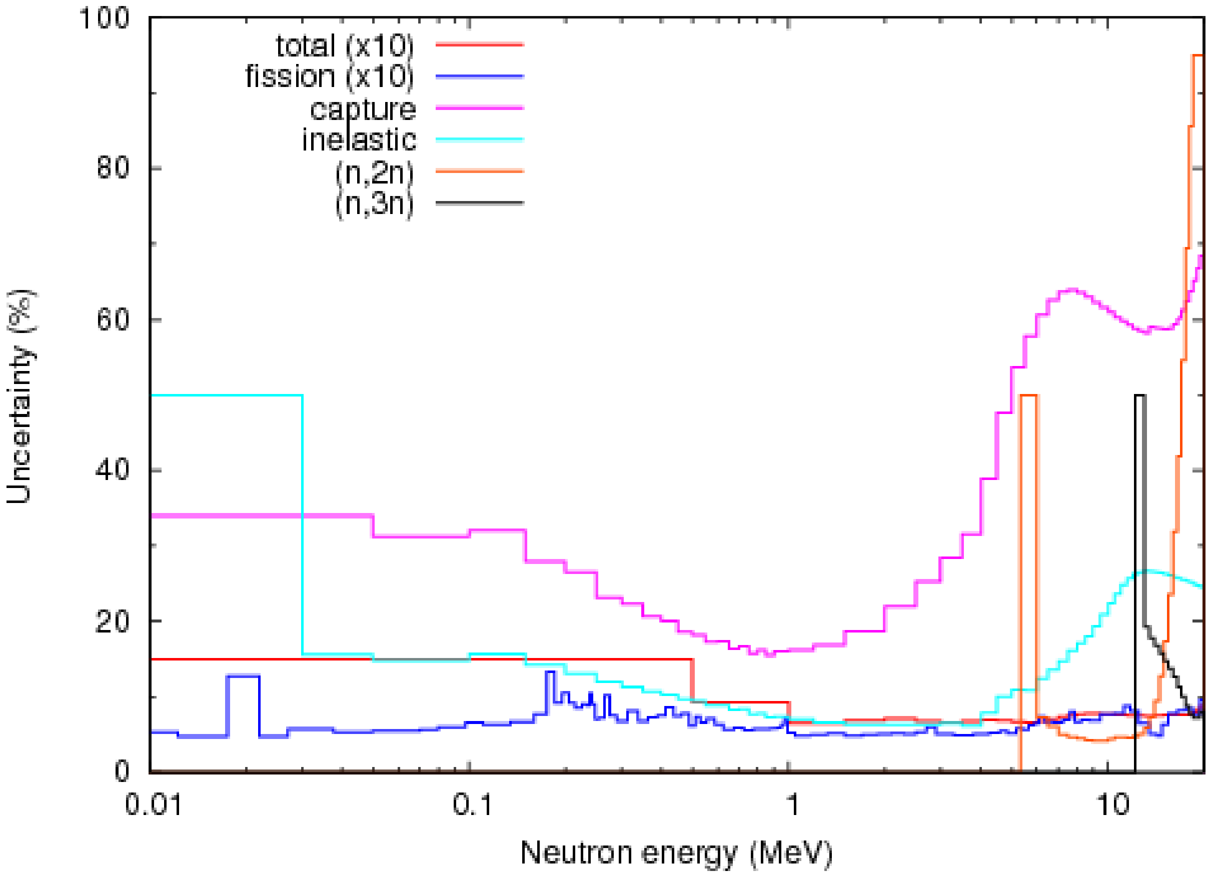
# Uncertainties in Group Structure



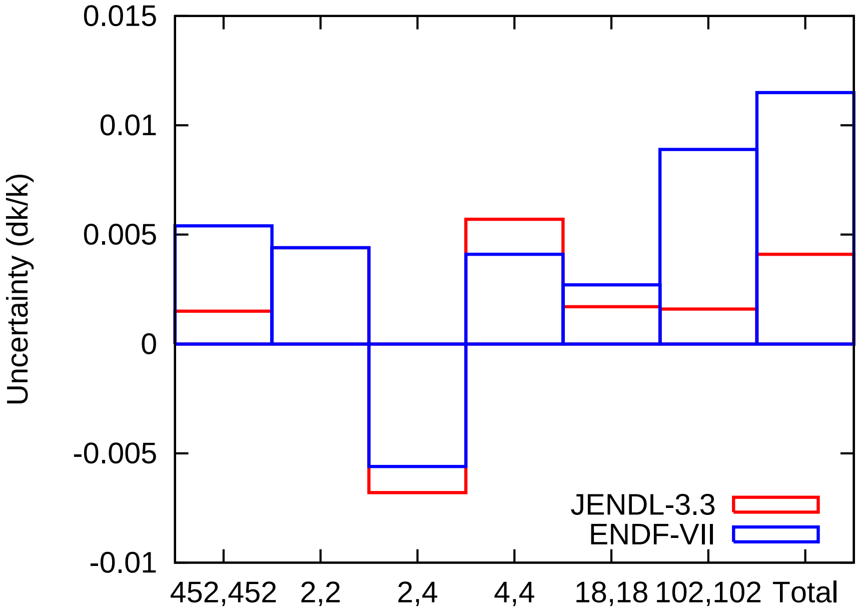

The evaluated covariance data were processed with ERRORJ (same as ERRORR in the fast region)

We observed that the grouped covariance depends on the group structure

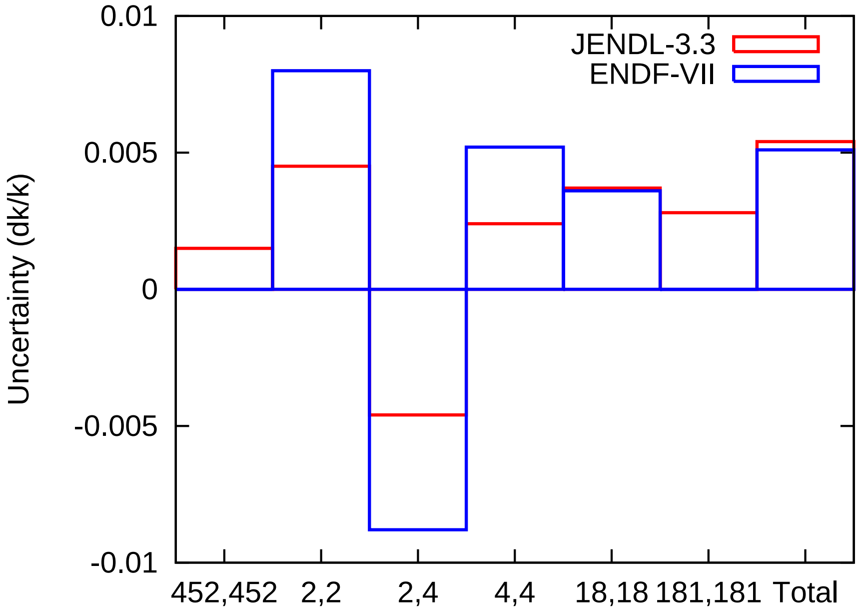
# Application of Covariance Data

## Uncertainty Calculation for LANL Critical Assembly

- The ENDF/B-VII covariance data were processed with NJOY to generate an 18 energy group library
- Sensitivities of the nuclear data to $k_{\mathrm{eff}}$ values for the LANL critical assemblies were calculated with the 1D $S_{\mathrm{N}}$ code, CBG/SNR (Chiba)




Godiva (U-235)




Jezebel (Pu-239)

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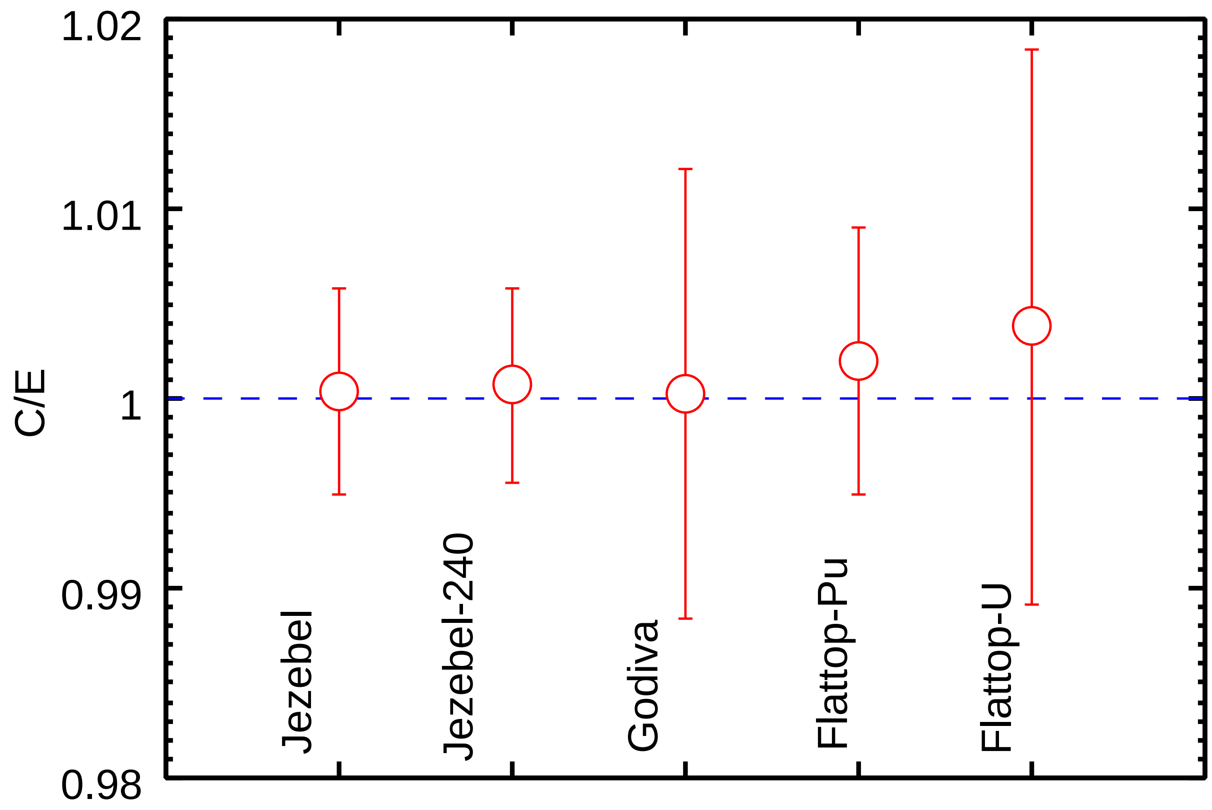
## Uncertainty Calculation for LANL Critical Assembly




Uncertainties taken into account for the calculated $k_{\mathrm{eff}}$ are, the nuclear data (covariance), experimental uncertainty in the integral data, and statistical error in the Monte Carlo method.

# Introduction

## Covariance Processing in the Resonance Region

- Covariances of grouped cross sections generated from a covariance matrix of resonance parameter
  - Reich-Moore resonance parameter covariance (SAMMY)
  - Compact format
- ERRORJ and PUFF can handle them

## New Development of ERRORJ

- Originally ERRORJ was started with the ERRORR module in NJOY
- ERRORJ was a stand-alone code. Users must use it with NJOY
- We remodeled ERRORJ such that one can used as a NJOY module
- Users can simply replace ERRORR in NJOY by ERRORJ
  - Covariance data in the entire energy range can be processed
- New version — more accurate and faster

# Covariance for Grouped Cross Sections

## Error Propagation from Resonance Parameters

Covariances of resonance parameters $V_{ij}$ are given in the ENDF files, where $i, j$ are the indices for the resonance parameters, $p$. The error propagation from the resonance parameter covariance to the grouped cross section covariance is given by:

$$\mathrm{Cov}(\sigma_a, \sigma_b) = \sum_{ij} \frac{\partial \sigma_a}{\partial p_i} \frac{\partial \sigma_b}{\partial p_j} V_{ij}$$

The sensitivity $\partial \sigma / \partial p$ can be calculated:

- With an analytical method — PUFF-IV
  - The SAMRML code was incorporated
- Numerical derivatives — ERRORJ
  - We stuck the same technique as before. However, the accuracy was checked against SAMRML.
  - The reasons are: more freedom for future development, and we do not expect any speed-up.

## Calculation Acceleration

The most time-consuming part is not a sensitivity calculation it self, but an energy integration over the energy grid.

**Old algorithm**

$$\frac{\partial \sigma_g}{\partial p_i} = \frac{\sigma'_g - \sigma_g}{\delta p_i}, \qquad \sigma_g = \frac{1}{\delta E} \int_{E \in g} \sigma(E) dE$$

**New algorithm**

$$\frac{\partial \sigma_g}{\partial p_i} = \frac{1}{\delta E} \int_{E \in g} \frac{\sigma'_g(E) - \sigma_g(E)}{\delta p_i} dE$$

where the perturbed $g$-th group cross section $\sigma'_g$ is calculated with the perturbed resonance parameter, $p'_i = p_i + \delta p_i$.

The revised algorithm is much faster than the old one, since $\sigma'_g(E) \simeq \sigma_g(E)$ when the $i$-th resonance is outside the group energy bin.

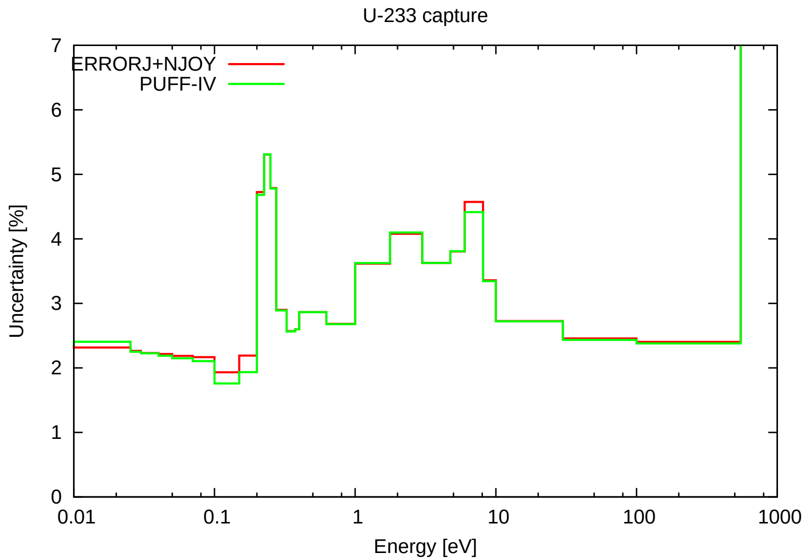
# Results

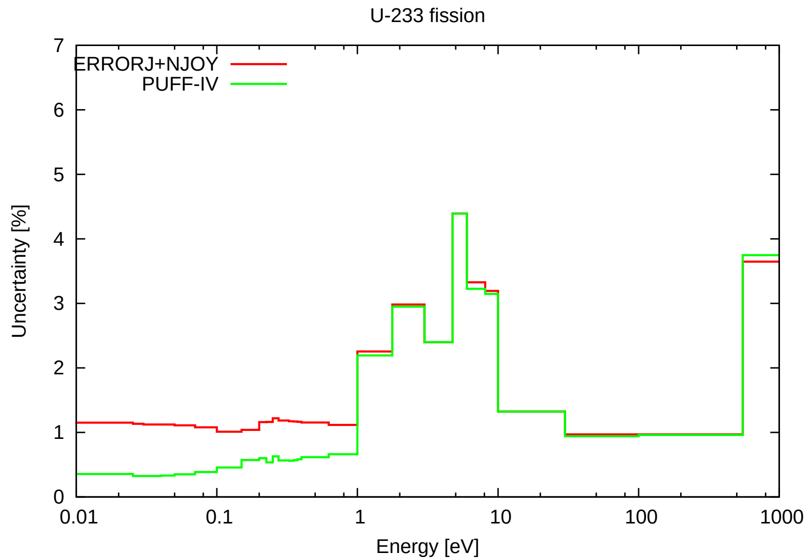
## How fast ?

| Processed nuclide | Original ERRORJ | Revised ERRORJ |
|---|---|---|
| U-235 (JENDL-3.2) | 2 hours | 40 min |
| Pu-239 (JENDL-3.3) | 3 hours | 50 min |
| U-238 (JENDL-3.3) | 12 min | a cup of espresso |
| U-233 (ENDF/B-VII) | Forever | 5 hours |

(Linux on Core Duo Laptop)

## Comparisons with PUFF-VI

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# Concluding Remarks

## Covariance Evaluation at LANL

- We evaluated the covariance data for major actinides : $^{235,238}$U and $^{239}$Pu in the fast region
- The GNASH-KALMAN method was establised, which runs on the T-16 Linux cluster
- The same technique will be used for other actinides, such as $^{233}$U and $^{241}$Am
- The evaluated data were processed with NJOY-ERRORJ to generate a grouped covariance, and uncertainties in the integral quantities were calculated

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