

# Covariances in the URR

Noah A. W. Walton & William N. Fritsch

D. Neudecker, A. Khatiwada, T. Kawano, A. Lovell, K. Fujio, M. Grosskopf

CSEWG 2025 11/05/2025

LA-UR-25-30698

# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.

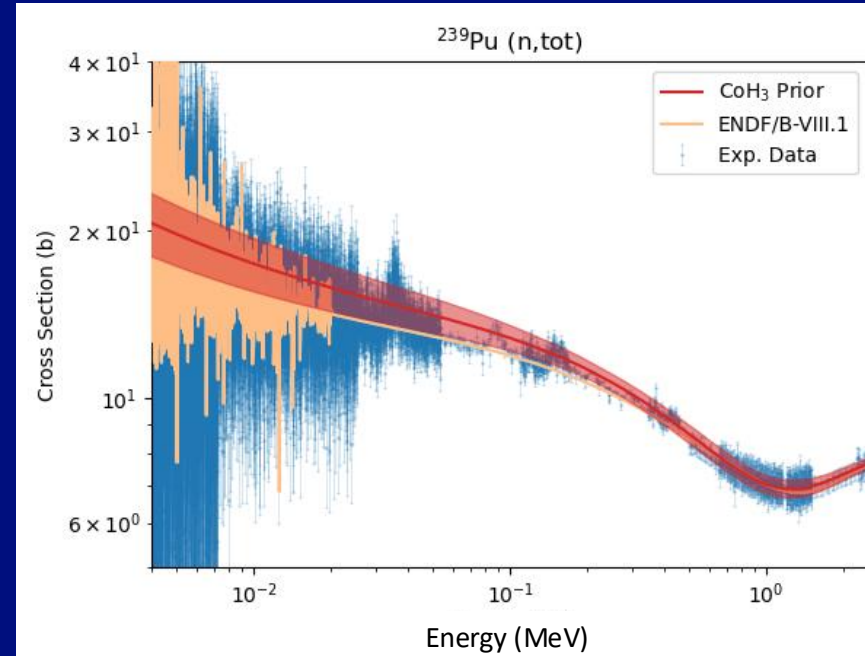


## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

1. ToF Uncertainty
2. How to average
3. PT Evaluation & Formatting



# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.

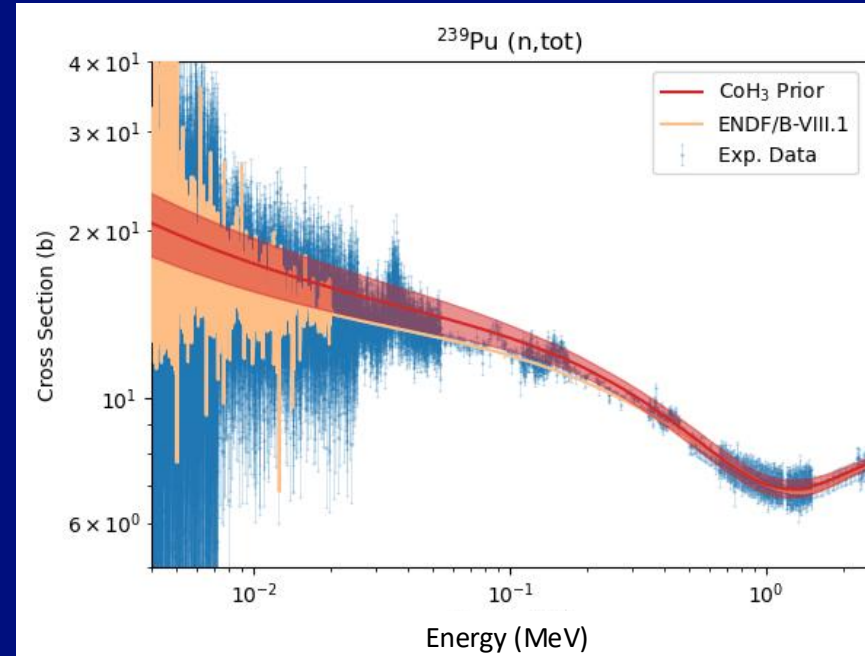


## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

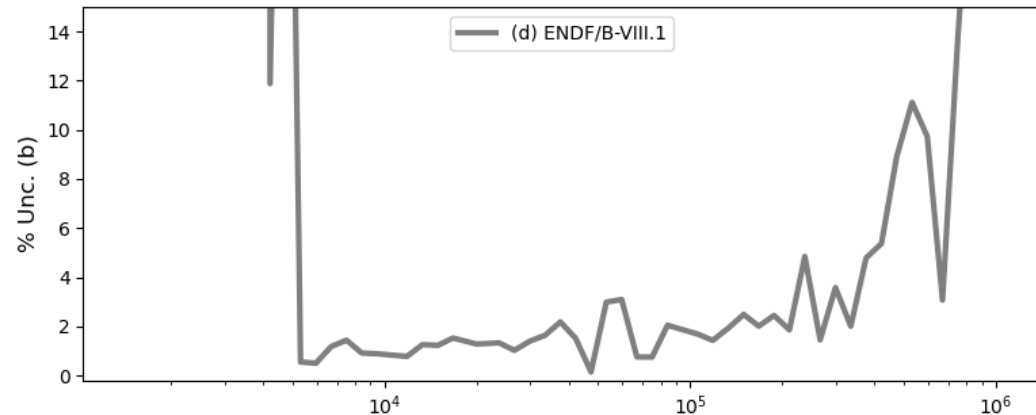
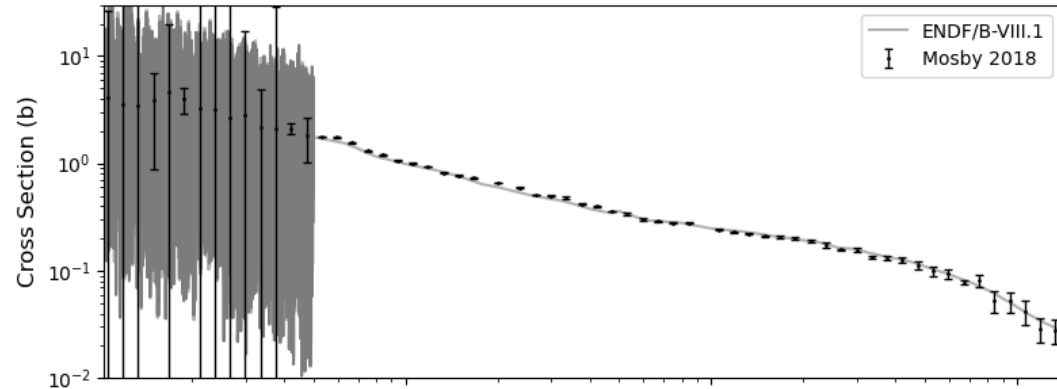
1. ToF Uncertainty
2. How to average
3. PT Evaluation & Formatting



# Consistent UQ w/templates across energy regions

Using ARIADNE Code @ LANL

## Pu-239 capture



ARIADNE: <https://doi.org/10.1051/epjn/2018012>

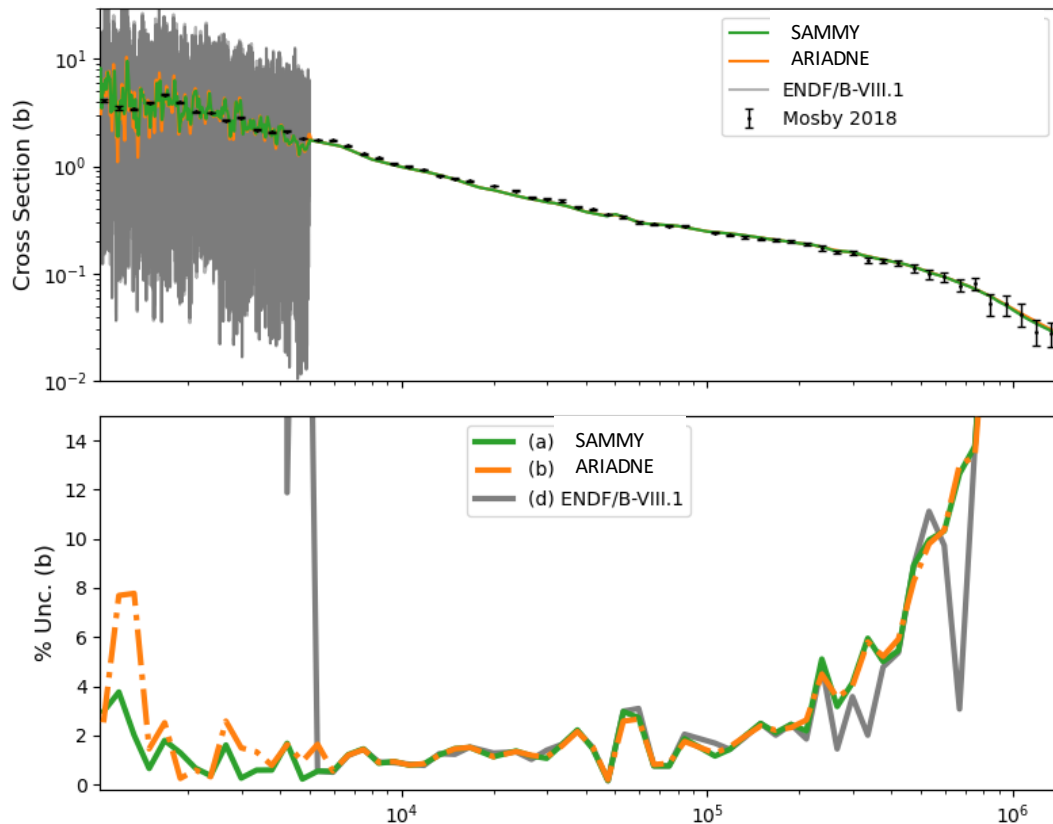
# Consistent UQ w/templates across energy regions

Using ARIADNE Code @ LANL

- Don't always have full resolution function
- Implemented broadening in ARIADNE UQ Code
  - Gaussian source
  - Channel/time bin width

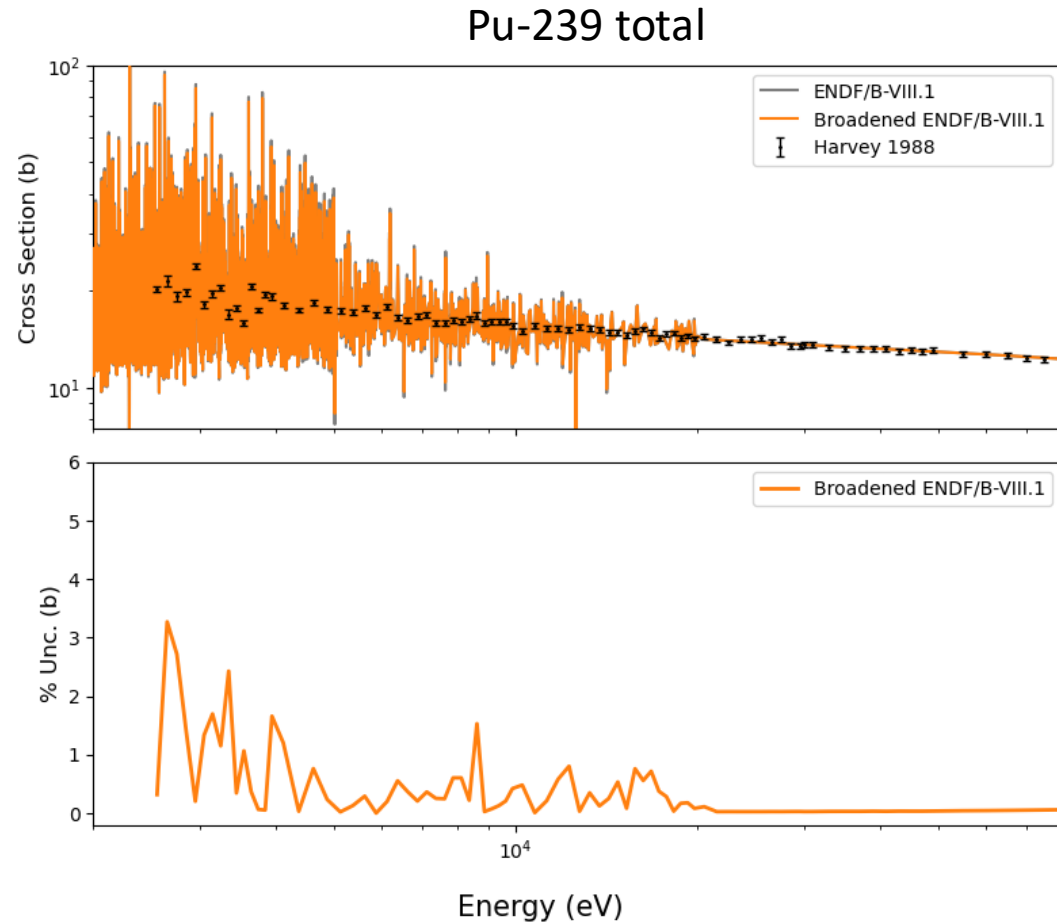
**Exact numerical agreement  
between codes if same  
resolution function**

## Pu-239 capture



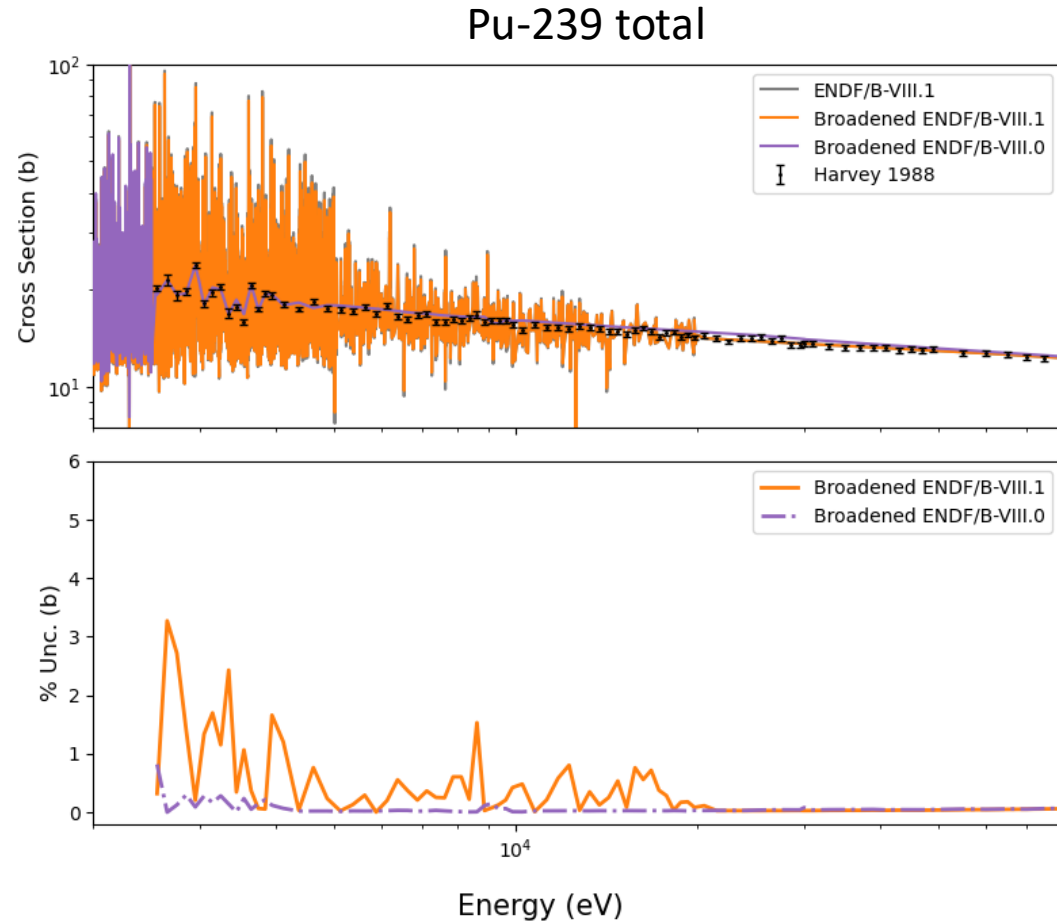
# Need RRR Model

- Approximate source and channel width broadening

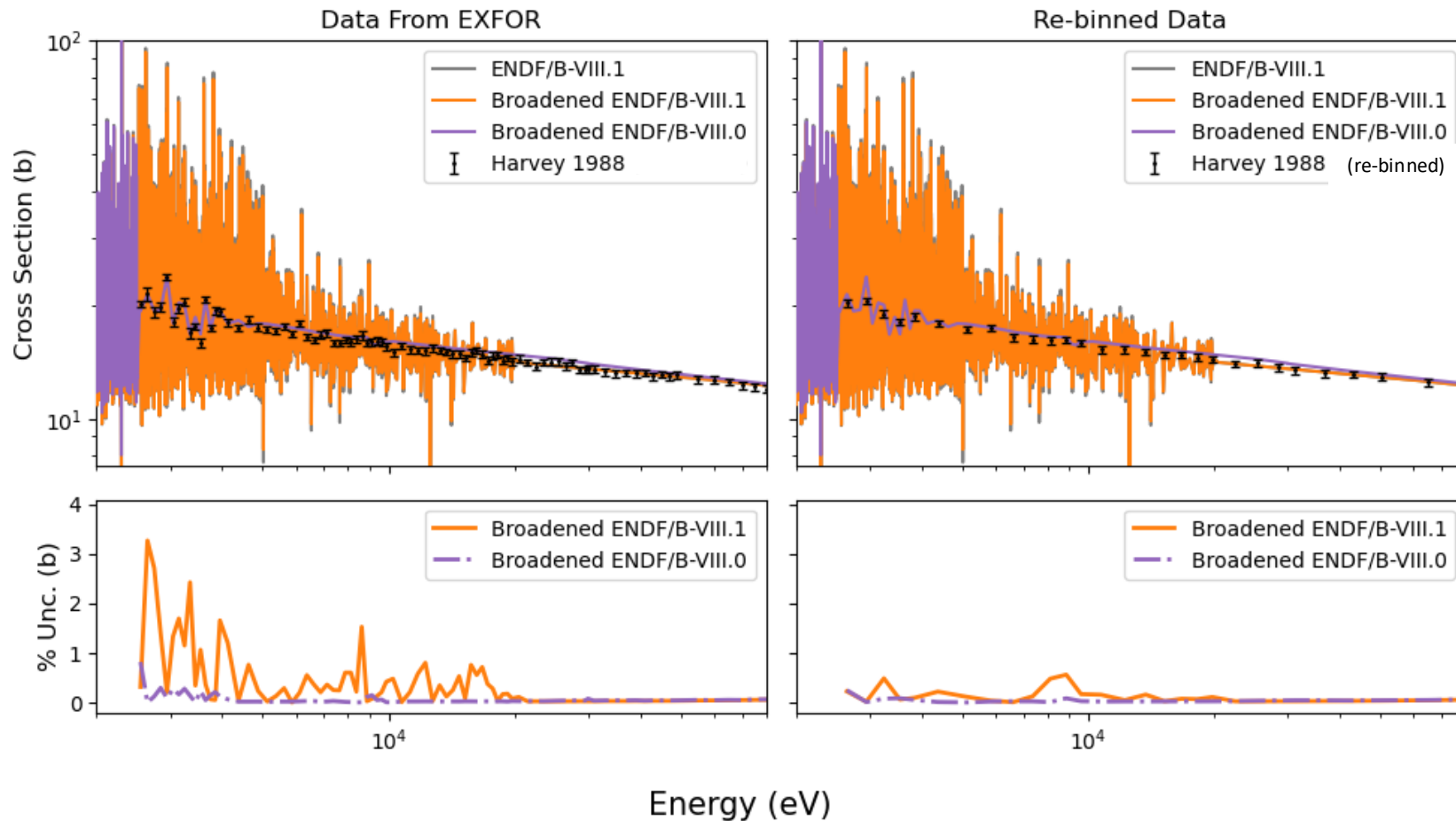


# Need RRR Model

- Approximate source and channel width broadening
- What if this was 2018?
  - The resonances go away!



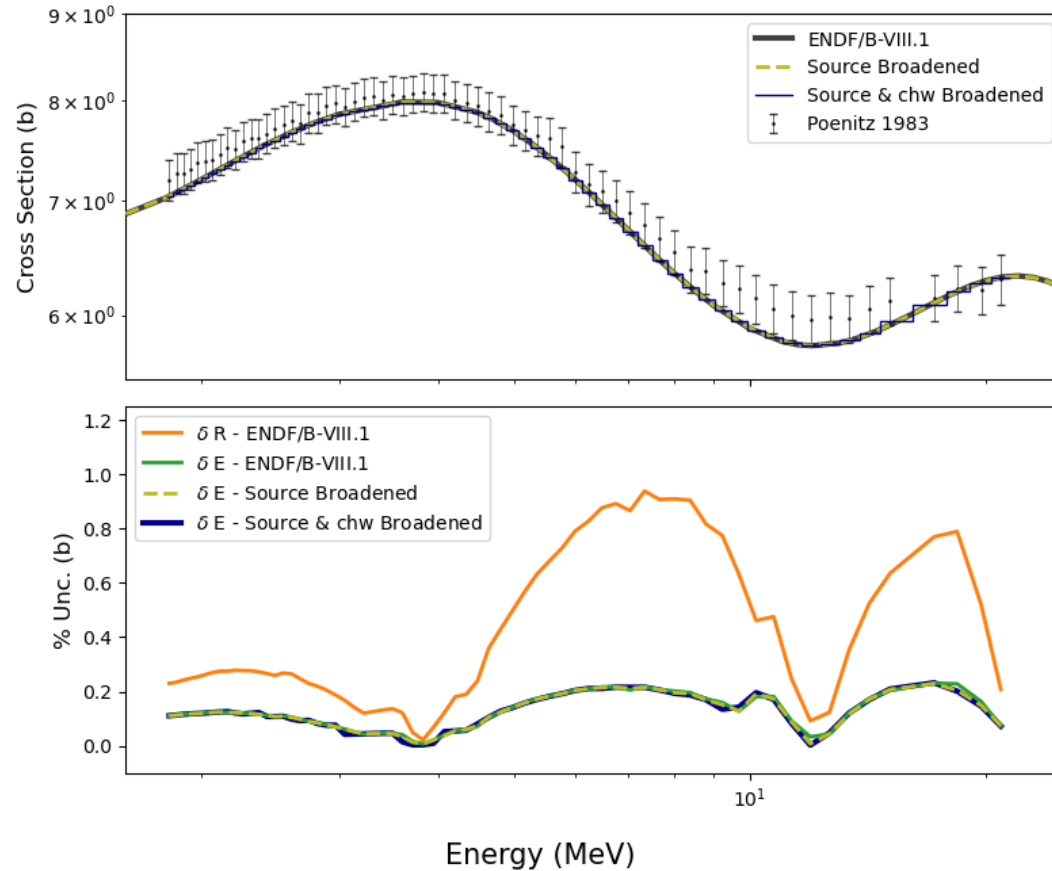
# Pu-239 total



# This still matters in the fast region!

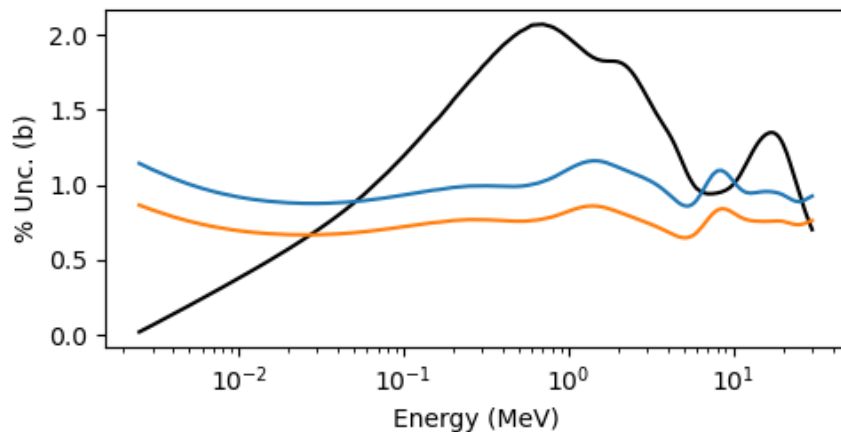
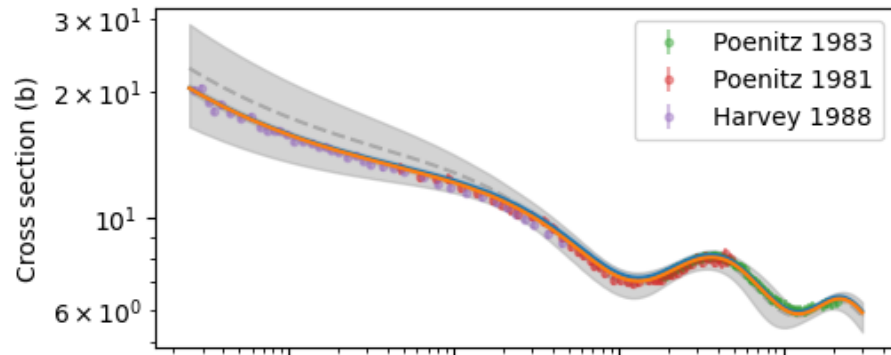
- Treating resolution as uncertainty is ‘conservative’ but not correct
- Model doesn’t change but UQ does

Pu-239 total

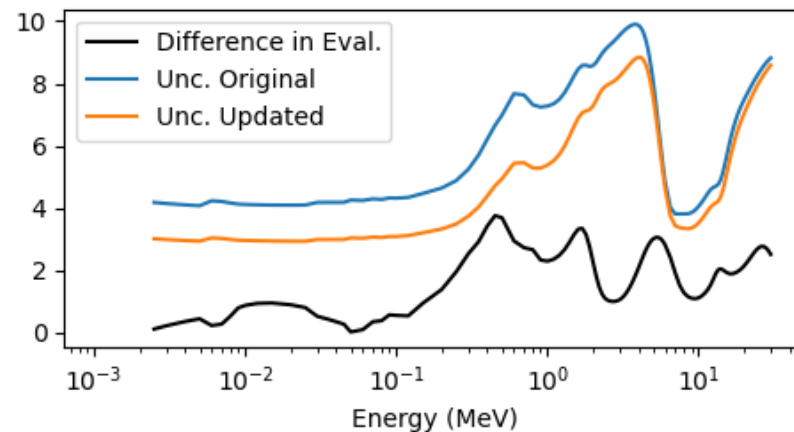
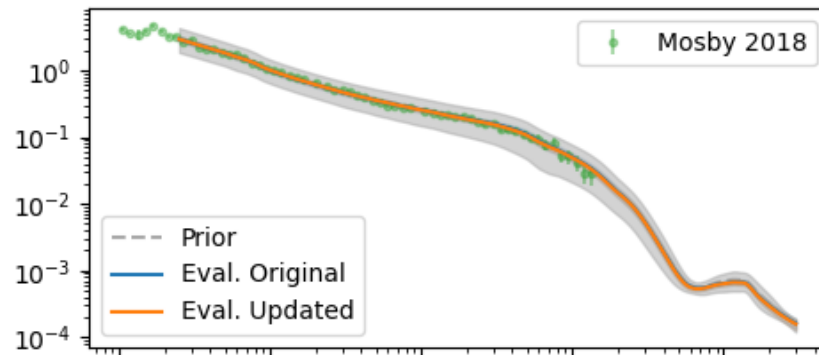


# Up to 2% difference in evaluated $\sigma$ and covariance

## Pu-239 total



## Pu-239 capture



# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.

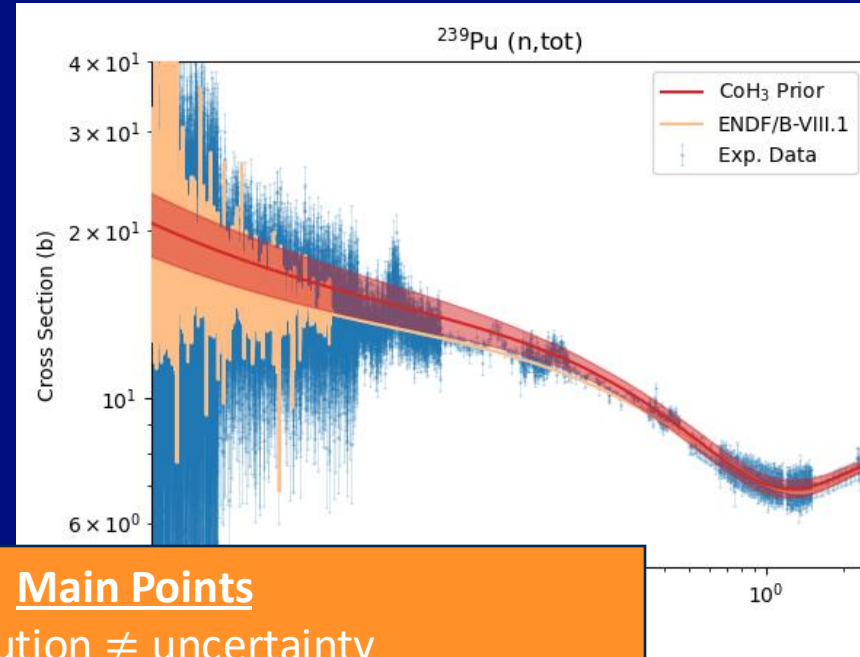


## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

1. ToF Uncertainty
2. How to average
3. PT Evaluation & Formatting



### Main Points

resolution  $\neq$  uncertainty  
data should represent average xs in URR  
re-bin data to correspond to underlying model

# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.

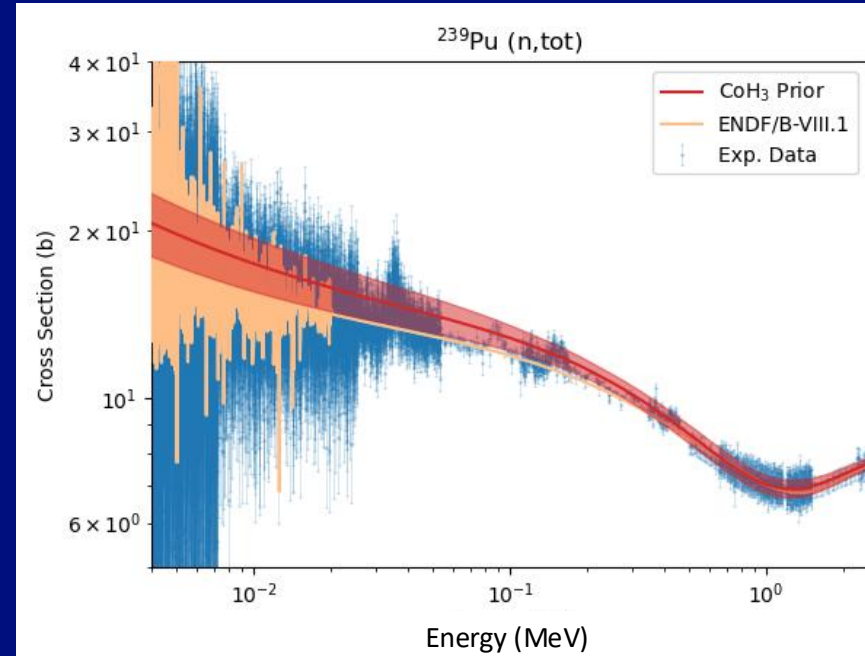


## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

1. ToF Uncertainty
2. How to average
3. PT Evaluation & Formatting



# How to Average Cross Sections in the URR

## Simple Average

$$\hat{\sigma} = \frac{1}{N} \sum_{i=1}^N \sigma_i$$

- Can be biased when uncertainty is present
- Includes moving filter averages
  - Savitzky-Golay

## Weighted Average

$$w_i = 1/\delta\sigma_i^2$$
$$\hat{\sigma} = \frac{\sum_{i=1}^N w_i \sigma_i}{\sum_{i=1}^N w_i}$$

- Same as regression to a flat function
- Cross sections are fluctuating so a flat function is a poor model

# How to Average Cross Sections in the URR

## Simple Average

$$\hat{\sigma} = \frac{1}{N} \sum_{i=1}^N \sigma_i$$

- Can be biased when uncertainty is present
- Includes moving filter averages

### Option 3:

Take larger counting bins

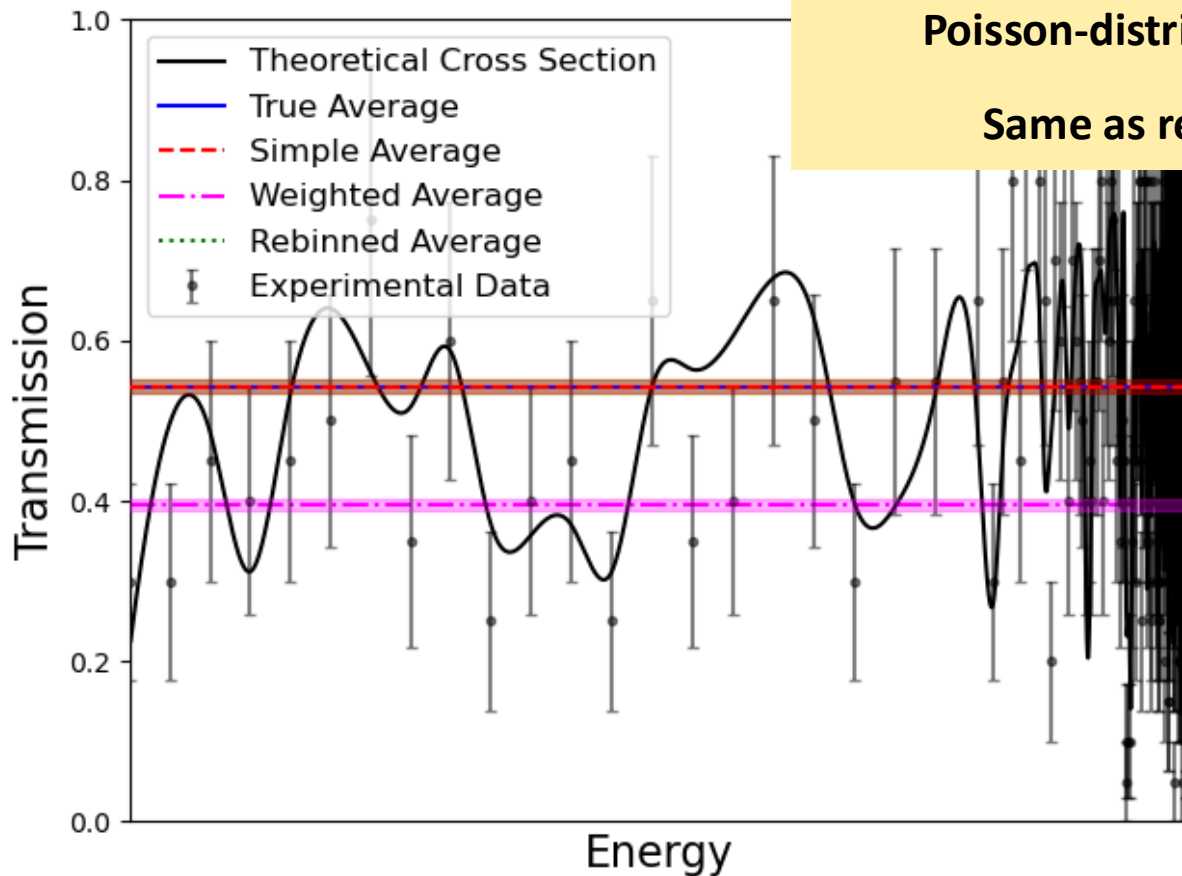
- Assumes you have raw count data

## Weighted Average

$$w_i = 1/\delta\sigma_i^2$$
$$\hat{\sigma} = \frac{\sum_{i=1}^N w_i \sigma_i}{\sum_{i=1}^N w_i}$$

- Same as regression to a flat function
- Cross sections are fluctuating so a flat function is a poor model

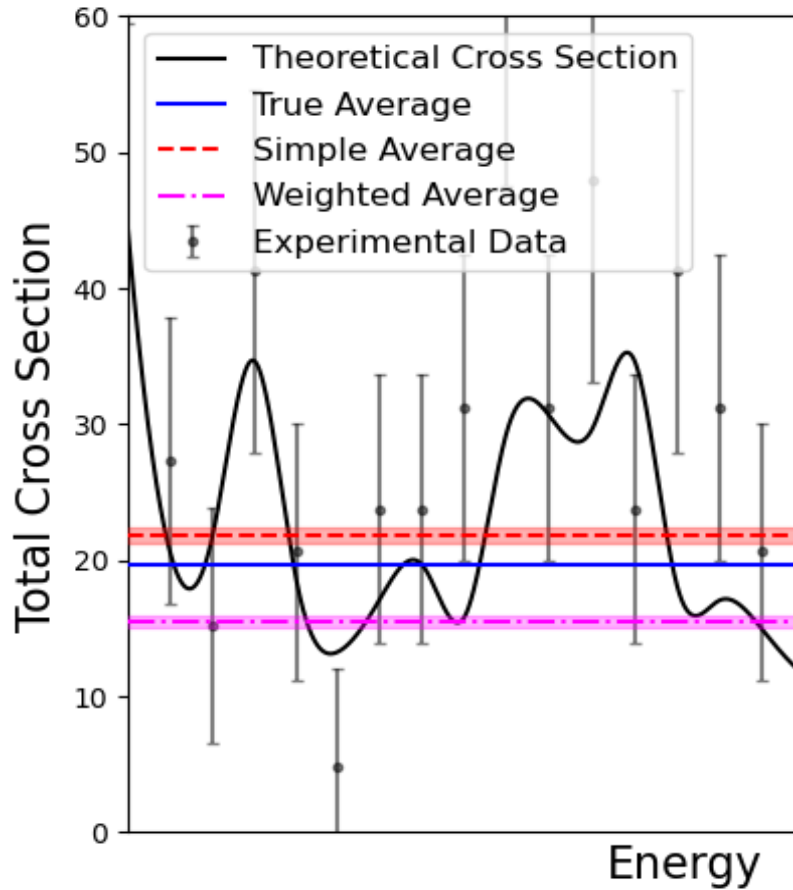
# Averaging in Transmission Space



Simple averaging is unbiased for Poisson-distributed data  
Same as rebinning

← Simple, Rebinned, and True Averages

# Averaging in Cross Section Space



$\sigma \sim \ln(\sigma)$   
Non-linearity = simple averaging fails!

This is not self-shielding!

# Criteria for Failure

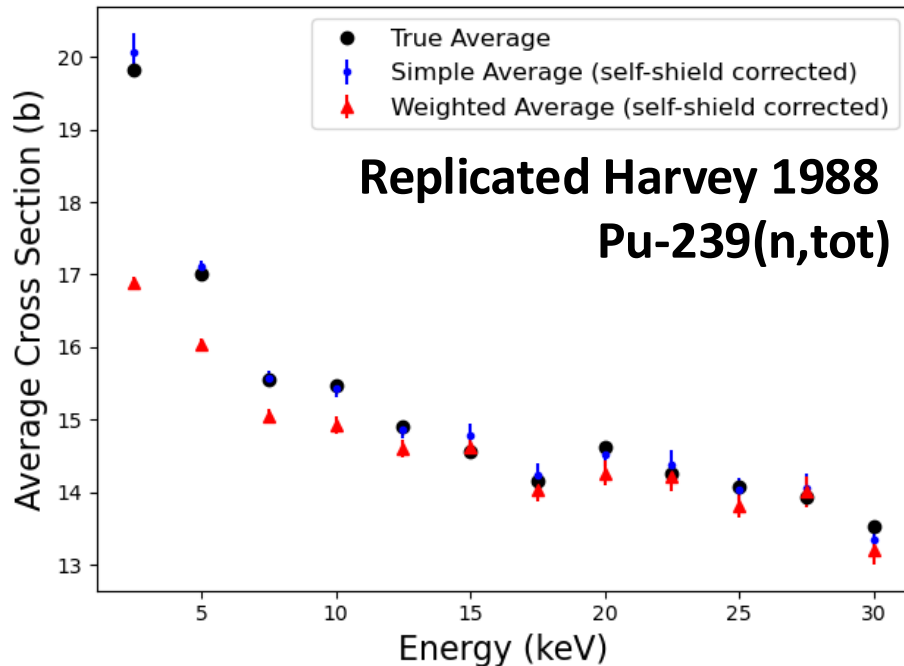
## Simple averaging fails when:

1. Data is highly stochastic, and
2. There is non-linearity with respect to the count data (i.e. self-shielding)

## Weighted averaging fails when:

1. The cross section fluctuates

*I would love to hear from URR cross section evaluators on the practice!*



# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.

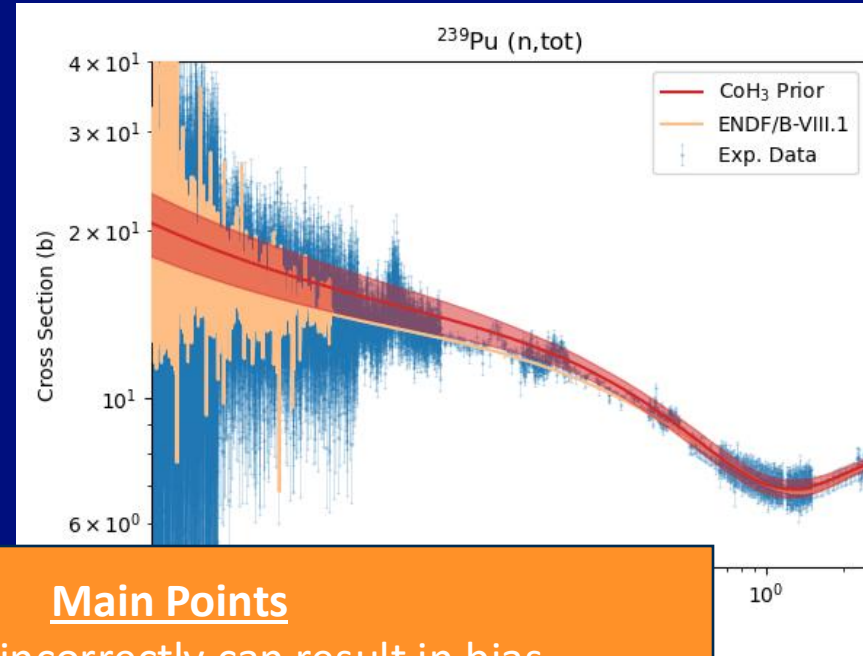


## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

1. ToF Uncertainty
2. How to average
3. PT Evaluation & Formatting



## Main Points

Averaging incorrectly can result in bias  
Rebin or Simple average in yield-space, not CS-space

# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.

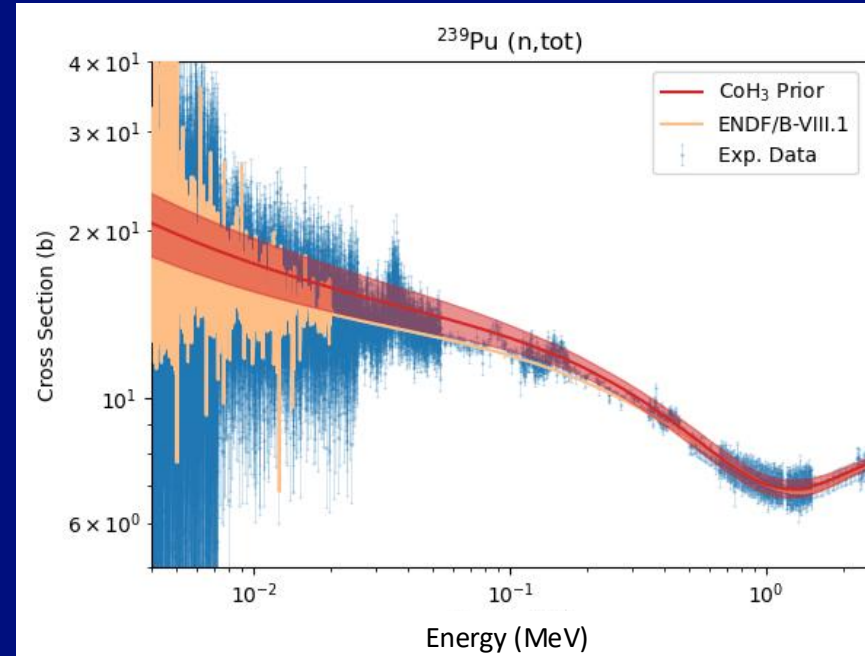


## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

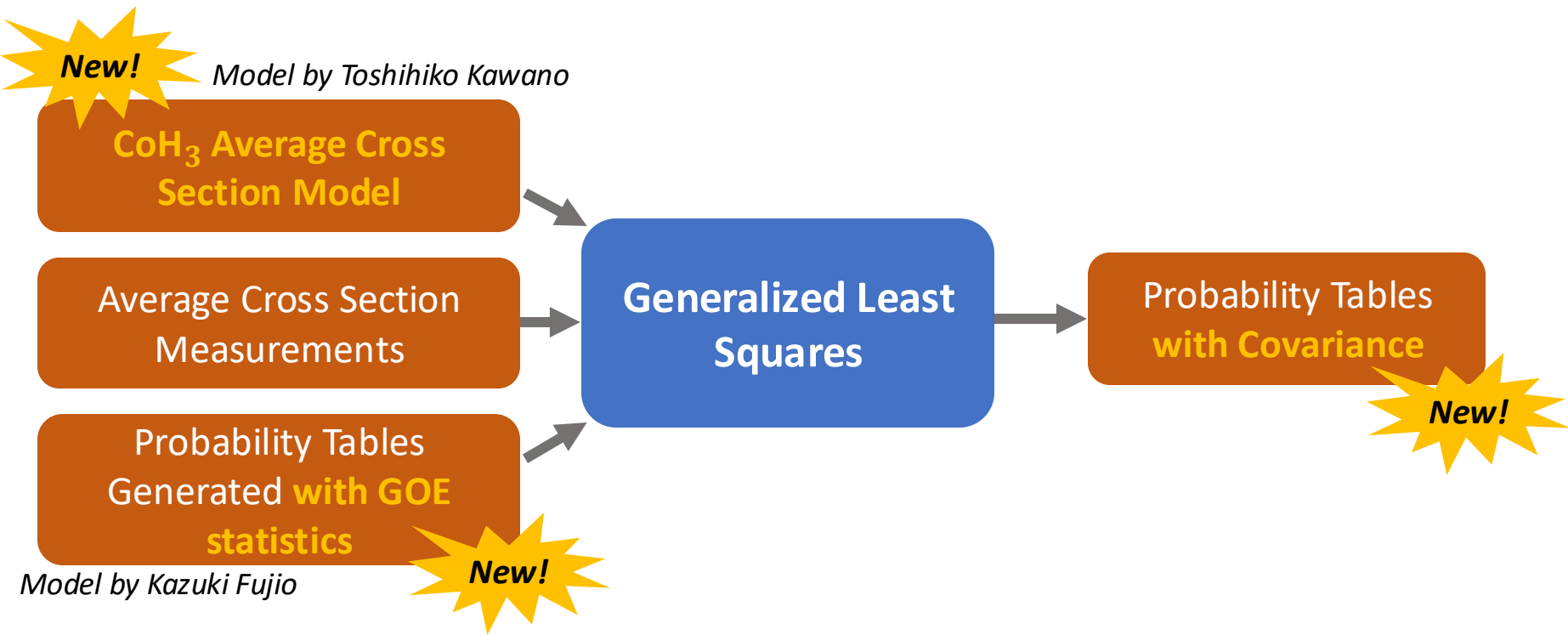
1. ToF Uncertainty
2. How to average
3. **PT Evaluation & Formatting**



# Probability Tables Informed by More Than Just Experiments



# Probability Tables Informed by More Than Just Experiments

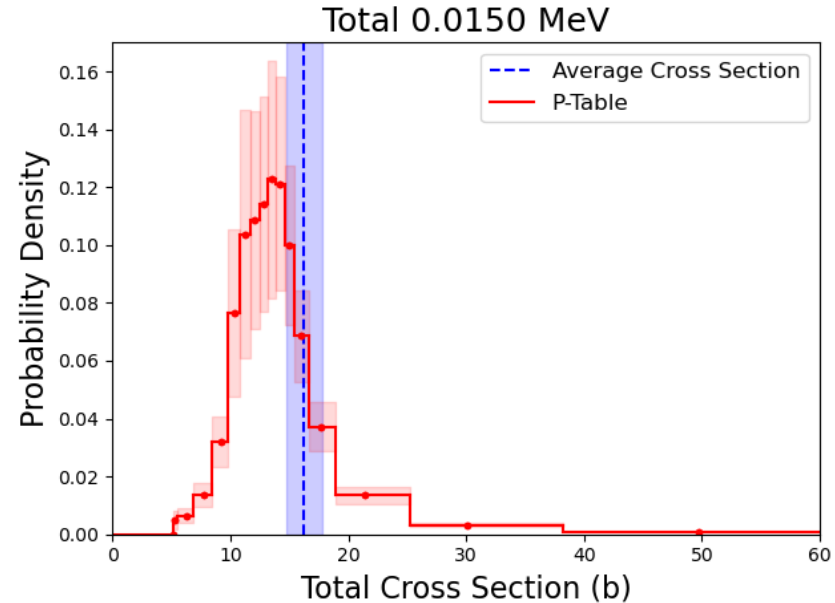


*More information on CoH<sub>3</sub>:  
Toshihiko Kawano, "Unified Coupled-Channels and Hauser-Feshbach Model Calculation for Nuclear Data Evaluation", 2019*

# How Do We Store Probability Tables and Uncertainty?

- **There is no ENDF format for P-tables or its uncertainty!**
- Could allow for transport unc. propagation (e.g. WHISPER) for P-tables
- Bypassing NJOY could allow P-tables informed by more than just average cross sections

## Probability Table with Unc.



# The goal of this work is to get evaluated covariances for PTables and from RRR-> fast.



## Goals

- Evaluate w/covariance across energy regimes (fast, URR, RRR)
- Probability table uncertainty/ covariance

## Challenges

1. ToF Uncertainty
2. How to average
3. PT Evaluation & Formatting



- Time-of-flight uncertainty is important for uncertainty quantification
- Resolution broadening is not an uncertainty, and should be treated separately
- Cross sections should be averaged in the URR to minimize fluctuations

- Evaluators should simple average in yield/transmission space to avoid bias

- We need an ENDF format for probability tables and covariance

# Acknowledgements



Research reported in this presentation was in part supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory under project number(s) 20240031DR and 20240878PRD4

Thank you, NEUP for funding support!

# Back Up Slides

# Why you need the CE resonance model

Consider the true (experimental) cross section to be  $\sigma(E)$ , but what is measured is actually

$$\sigma'(E) = \frac{\int_{E-a}^{E+b} \sigma(E) dE}{a+b} \quad (1)$$

$$\equiv \frac{\int \sigma(E) dE \Big|_{E+b} - \int \sigma(E) dE \Big|_{E-a}}{a+b} \quad (2)$$

This applies only if the bin width integration is NOT already baked into  $\sigma(E)$  from broadening. The uncertainty in energy should be propagated to the model of what is measured,  $\sigma'(E)$ , not  $\sigma(E)$ . The first order linear propagation will then use the derivative of  $\sigma'(E)$

$$\frac{\delta}{\delta E} (\sigma'(E)) = \frac{\delta}{\delta E} \left( \frac{\int \sigma(E) dE \Big|_{E+b} - \int \sigma(E) dE \Big|_{E-a}}{a+b} \right) \quad (3)$$

$$\equiv \frac{1}{a+b} \left[ \frac{\delta}{\delta E} \left( \int \sigma(E) dE \Big|_{E+b} \right) - \frac{\delta}{\delta E} \left( \int \sigma(E) dE \Big|_{E-a} \right) \right] \quad (4)$$

$$\equiv \frac{\sigma(E+b) - \sigma(E-a)}{a+b} \quad (5)$$

# Applied UQ templates

Using ARAIDNE Code @ LANL

- Overestimated uncertainty in lower energy ranges
- Narrowed down the issue to TOF/energy uncertainties
- Need a model of the experiment

**Exact numerical agreement  
between codes**

# Consistent with RRR

Using SAMMY code @ ORNL

- Both regimes use first order propagation onto data covariance matrix
  - $\Delta y^2(\Delta E) = \left(\frac{\partial y}{\partial E} \Delta E\right)^2$
- Integral over experimental bins is in resolution broadening function
  - Other experimental corrections should be included in  $y$ , but width of bins dominates at higher energy

# ENDF Manual Statement

The following caution should be noted by evaluators in choosing this option:

Because File 3 is energy varying, it inherently has the possibility to energy-self-shield itself. If File 2 also shields it, one may actually "double-shield". The problem will probably be most acute just above the boundary between the resolved and unresolved regions, since the experimental resolution may still be good enough to see clumps of only a few resonances.

One might consider "correcting" for this in the choice of File 2 parameters, but this would be difficult because the degree of shielding is application dependent. A better procedure would be to insure that each significant structure in File 3 actually represents a statistically meaningful number of resonances, say ten or more. If the raw data do not satisfy this criterion, then additional smoothing should be applied by the evaluator to make it a correct condition on the data. A careful treatment will require the use of statistical level theory to determine the true widths and spacings underlying the File 3 structures.

# Probability Tables with Uncertainty

