Applying (n,tot), scattering and capture templates and new database

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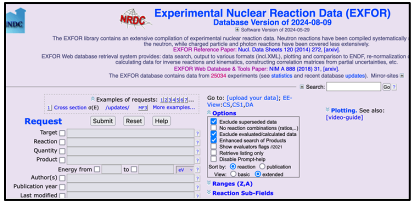
Background

1. It's been well-established as a community the importance of having trustworthy uncertainties from data (and theory models) for reliable ND evaluations.

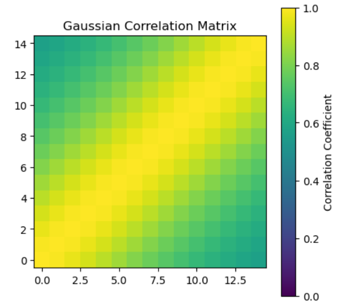
2. The templates of experimental uncertainties from CSEWG provide some guidance for experimentalists in reporting uncertainties and for data evaluators to estimate missing/under-reported uncertainty sources by the experimentalists.
   - Particularly useful when the EXFOR database is incomplete, inconsistent, authors cannot be contacted, etc.
   - Example cases from two projects: propagation of ND uncertainties for LANL applications & LANL LDRD-DR project: PARADIGM (focus on n,tot).

3. Use of templates does not eliminate the need for careful considerations of many parameters and subjective evaluation of factors that went into making those experimental measurements.

Workflow



CSEWG exp templates



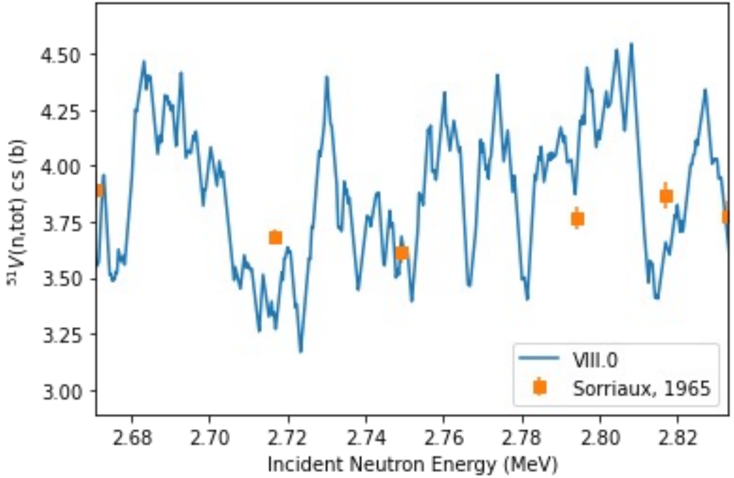
ARIADNE for UQ (fast region)

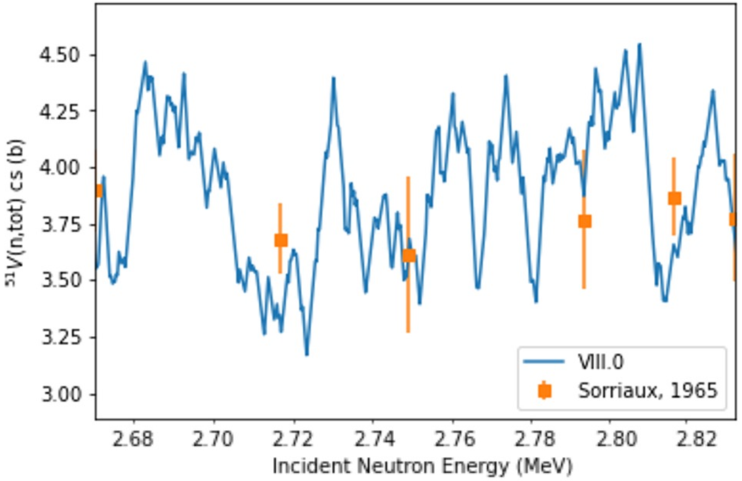
EPJ-N 4, 34 (2018)

- Careful parsing of EXFOR data and any associated documents
- Documentation of features (hardware, experimental method, bibliography, corrections, etc.)
- Documentation of the provided uncertainties, their sources, and optional correlations
- Accept/Reject data based on the available information
- Fill missing uncertainties
- Construct correlation matrix associated with each uncertainty source
- Construct full covariance matrix and estimate total uncertainty
- Store data in a .json format

Example case from V-51 (n,tot)

- Currently no covariances exist for V-51 in ENDFB-VIII.0.
- "Total" uncertainties from EXFOR make data look like outliers (left).
- More detailed UQ (right) shows data are consistent with evaluation.
- Includes sample mass and energy resolution unc. (not part of total EXFOR unc.) but given by experimenters and some template uncertainties.





Template Uncertainty (n,tot)

TOF

Uncertainty source		Unc. (%)	Corr. (i,j)
ΔE			Strong Gaussian
δn		See Table 3	Fully
$\delta \dot{c}$			Uncorrelated
$\delta \dot{b}$			Uncorrelated
δK	(saturated res.) (w/o saturated res.)	3 5	Fully
$\delta \dot{B}(t)$			Strong Gaussian
δN_T	(with cycling) (w/o cycling)	1–2 2–6	Fully
δF_T			Strong Gaussian

Sample type	δn (%)
Metal	0.1–1
Powder	2–5
Liquid	0.1–1
Diluted liquid	2–5

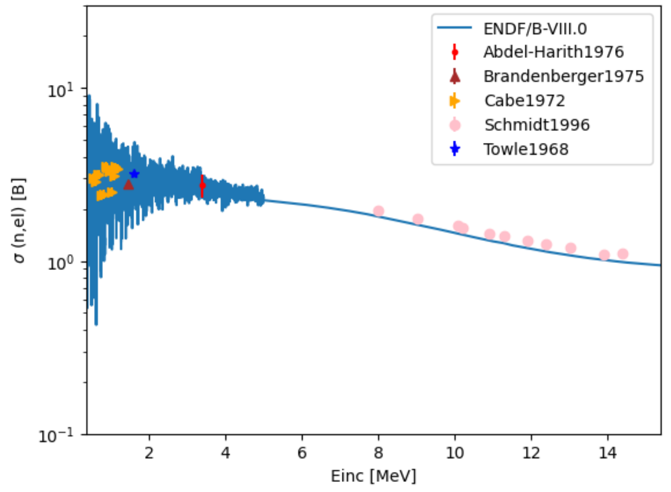
Mono-energetic

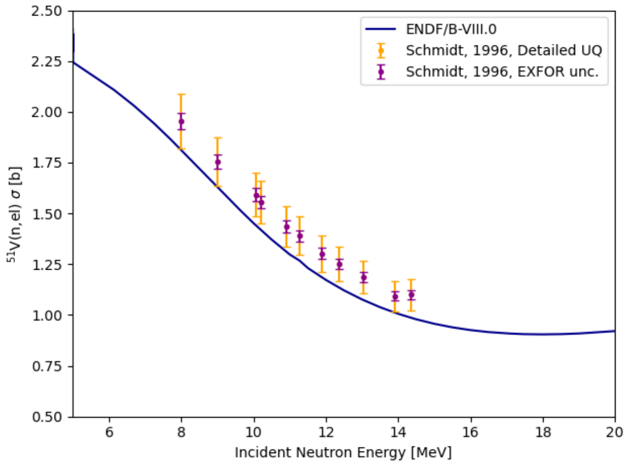
Uncertainty source	Unc. (%)	Corr. (i,j)
ΔE		Strong Gaussian
δn	See Table 3	Fully
δc		Uncorrelated
$\delta \Delta T$	20	Strong Gaussian
$\delta \beta$		Fully
$\delta \gamma_1$, $\delta \gamma_2$, $\delta \zeta$		Strong Gaussian
δN_T		Uncorrelated

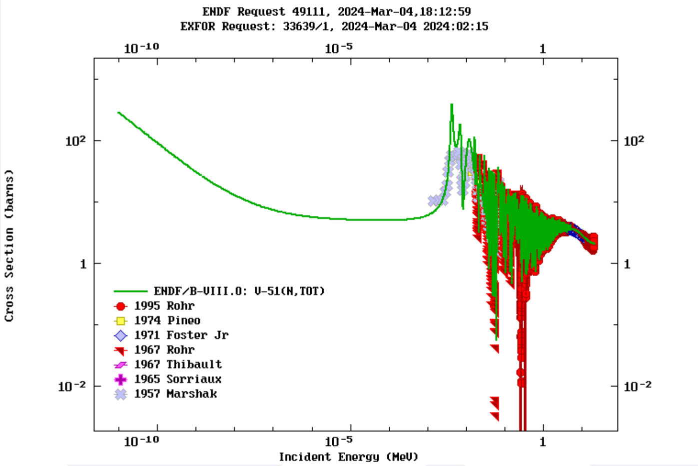
- Uncertainties that are provided in the templates are w.r.t the respective parameters, need to account for the sensitivities when propagating to uncertainty on cross-section (exp dependent).

V-51 (n,tot) and (n,el) UQ

- With a little bit of care, the UQ was straight-forward and the impact is clear.
- 2/5 (n,el) and 3/7 (n,tot) data accepted.
- LANL T-2 colleagues performed new V-51 evaluation based on these experimental data







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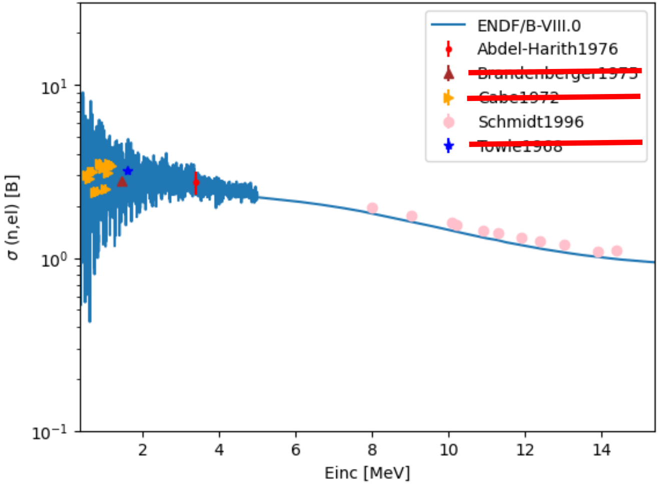
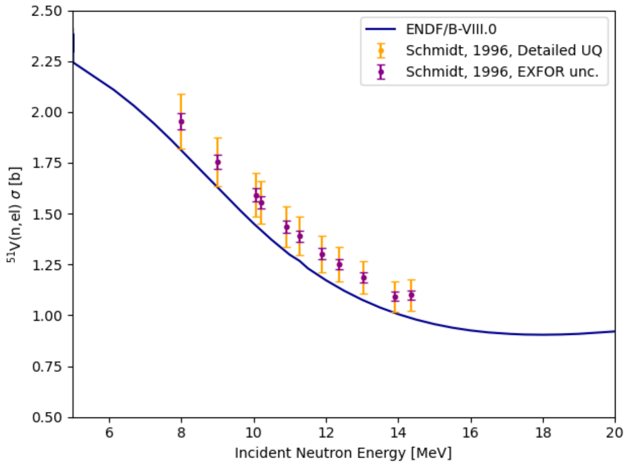
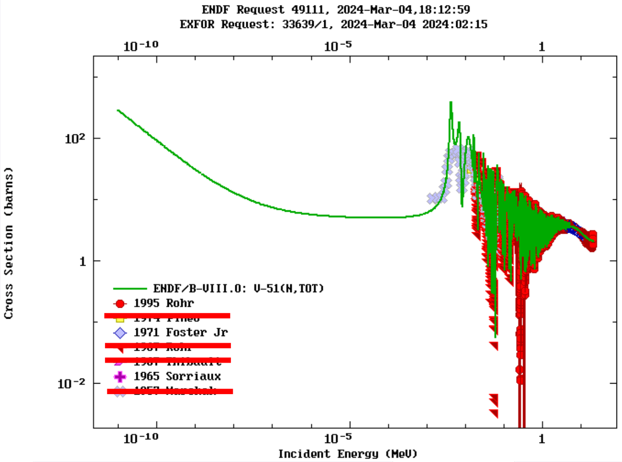
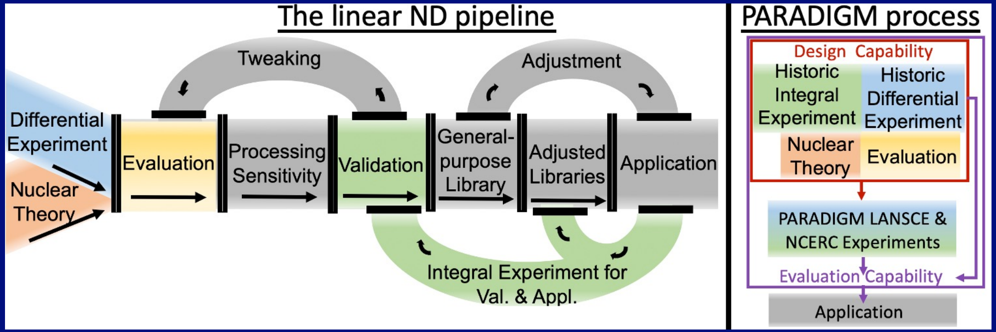




Rejected mostly for not having enough unc. info & proper documentation to apply template



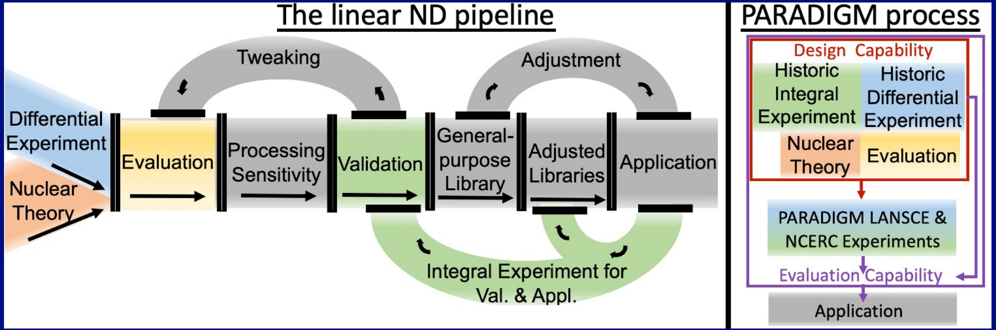
Example case of Pu239 (n,tot) UQ for PARADIGM



PARADIGM project combines information from differential and integral experiments in parallel to best reduce ND uncertainties applicable for various applications in the 1-600 keV range.

Example case of Pu239 (n,tot) UQ for PARADIGM

- Full covariance information on differential data can provide complete information that treating these dataset as independent points doesn't.
- However, the underlying assumptions for constructing covariance matrices using the templates need to be respected and thoroughly considered.



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Schwartz1974 Pu239 (n,tot)

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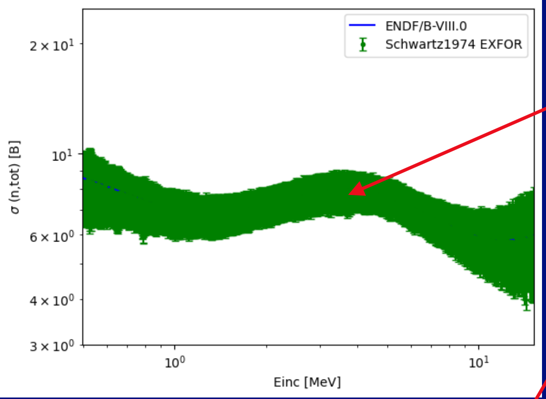

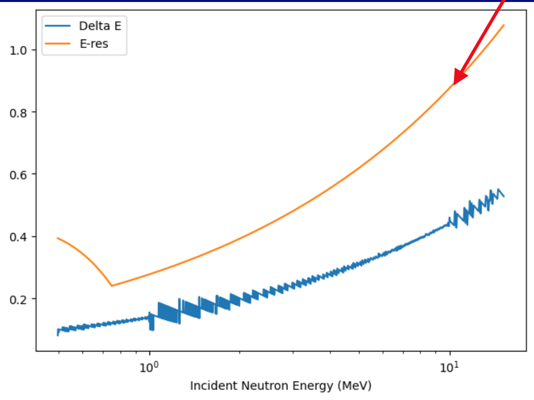

- 1680 very finely binned data points
- Reported energy resolution of the measurement is larger than the estimated bin-width.
- Therefore, the measured counts/transmission in each bin are expected to be anti-correlated to the counts in the adjacent bins

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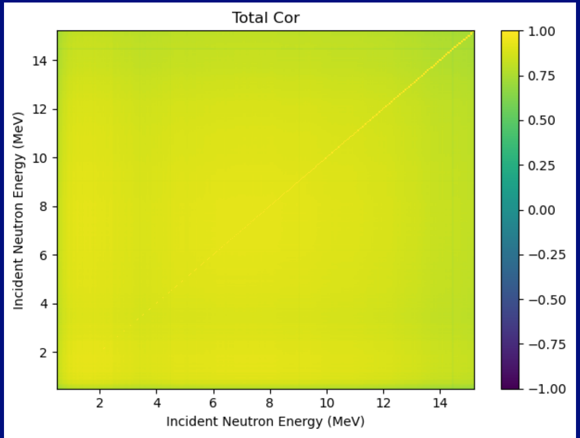
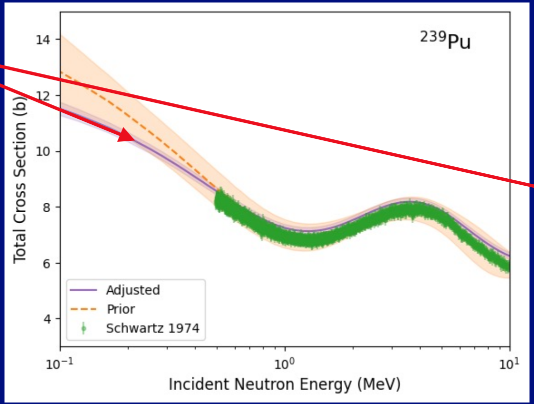
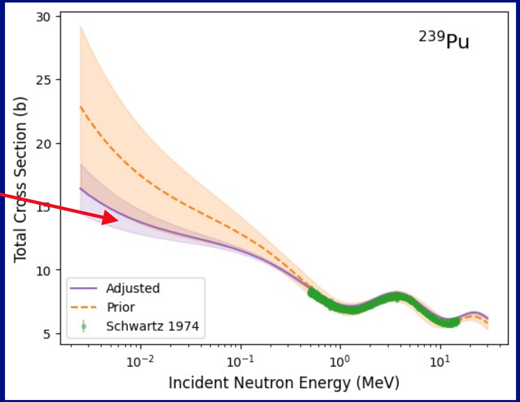
Schwartz1974 Pu239 (n,tot)

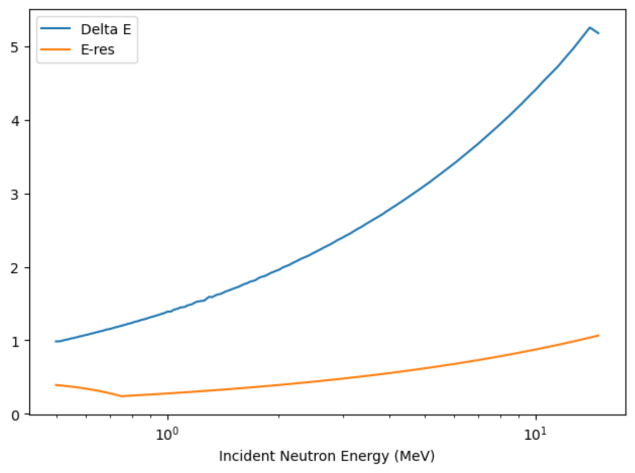
- Template assumes uncorrelated uncertainty due to counts.
- Unbinned data is too rigid (high correlation across incident neutron energy bins).
- Pulls the adjustment away from the theory prior at lower energies.
- Assuming independent datapoint, adjustment moves in expected direction.







Schwartz1974 (n,tot)



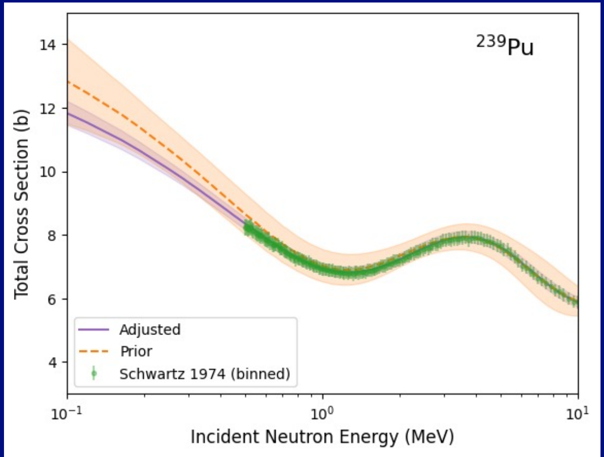
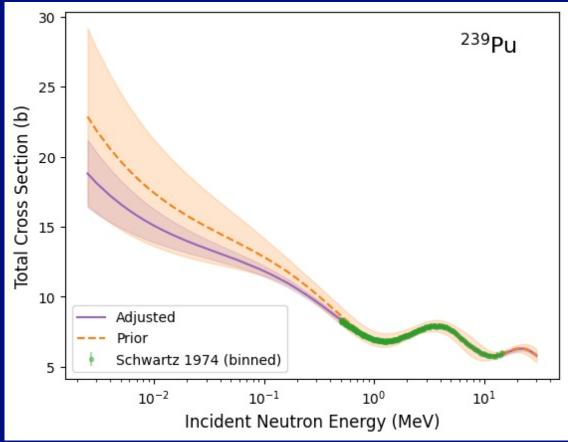


Figure for illustration only, doesn’t have other experimental data

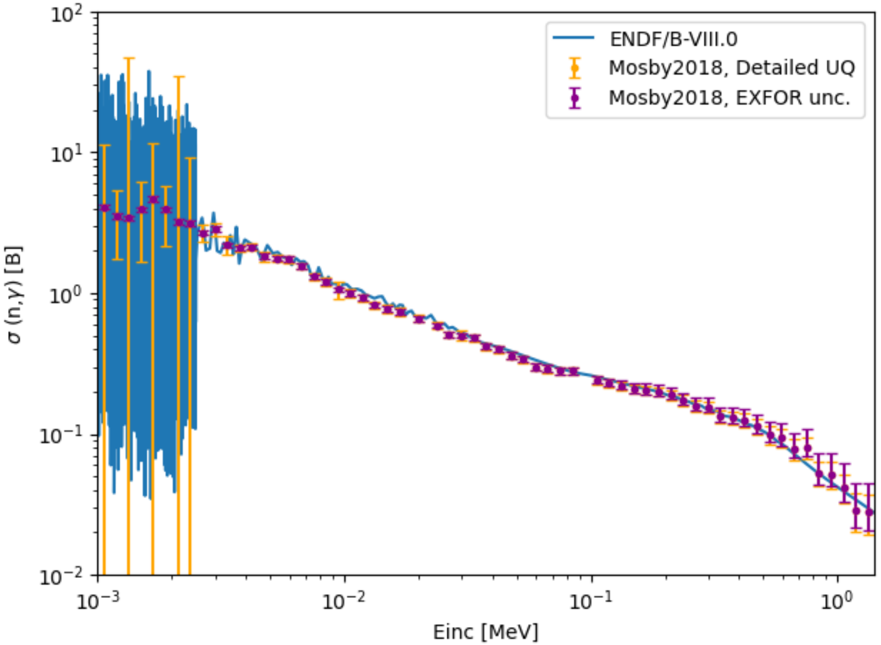
Rebinning the data so that the energy bin width is larger than the energy resolution fixes the issue.



Bridging the gap between different energy regions

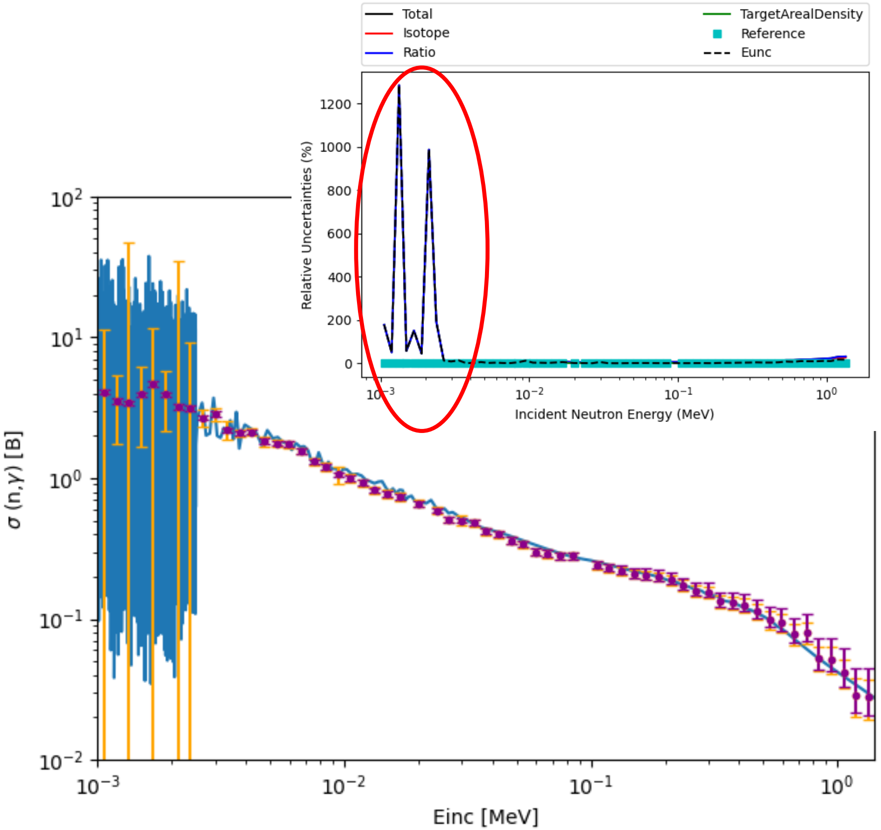
- PARADIGM project deals with applications in the intermediate energy range (1-600 keV).
- ARIADNE code was originally developed by Denise Neudecker for the experimental UQ of prompt fission neutron spectra in the fast energy region.
- Since then, we've expanded the code to include many other observables and also pushed the capability in the intermediate energy region.

Data sometimes span large order of magnitude in energy



Bridging the gap between different energy regions

- Minimal input from template uncertainty.
- Only slight change in the fast region, but significant increase in total uncertainty (coming from how energy resolution is propagated) in the medium energy range.
- The methodology to propagate uncertainty/resolution in incoming neutron energy to the cross-section using past evaluations works well for smooth regions in fast range but break in the regions with rapidly fluctuating cross sections.
- Open question: how to seamlessly merge the UQ methods in RRR regions to those in fast regions to properly quantify uncertainties in URR?



Conclusion

- CSEWG templates for experimental UQ have been useful to provide guidance for filling out estimate missing/under-reported uncertainties and experimental covariances for multiple projects at LANL.
- New V-51 evaluations were done using data UQed using these templates.
- Performed experimental UQ using the templates for a large suite of nuclei and observables for PARADIGM project.
- Experience of using the templates suggests need for continued careful consideration of the assumptions made for the suggested values & correlations in the templates, experimental parameters, measurement types etc. while using them.
- Community discussion on how to best combine methods for UQ at different energy regime is needed.

Acknowledgement

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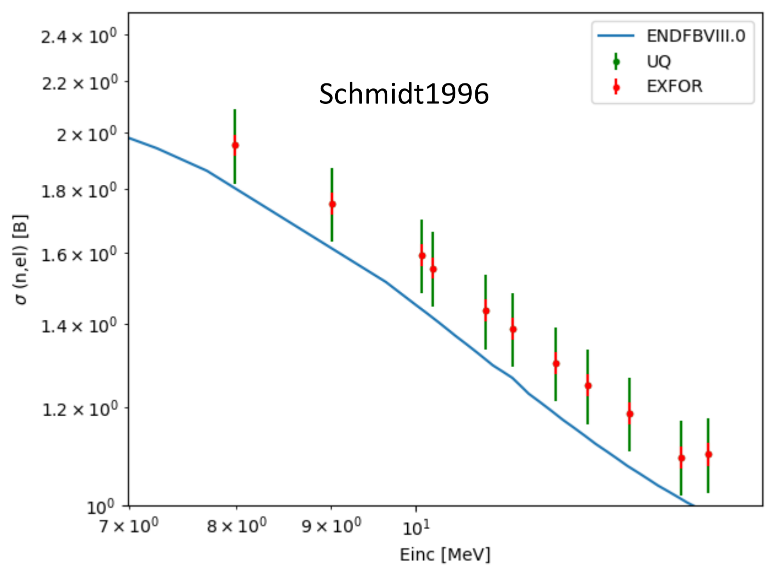
Template Uncertainty Method

- What?
  - CSWEG came up with templates for estimating experimental uncertainties for various reactions/observables in order to standardize/provide recommendations for experimentalists in reporting uncertainties and for data evaluators to estimate missing/under-reported uncertainty sources by the experimentalists.
  - Separate templates exist for different reactions
    - General paper: https://doi.org/10.1051/epjn/2023014
    - neutron-induced total: https://doi.org/10.1051/epjn/2023018
    - (n,γ) and charged-particle: https://doi.org/10.1051/epjn/2023015
    - Prompt fission neutron spectra: https://doi.org/10.1051/epjn/2023013
    - (n,xn) reaction cross section: https://doi.org/10.1051/epjn/2023019
    - average prompt and total fission neutron multiplicities: https://doi.org/10.1051/epjn/2023016

Template Uncertainty Method contd..

- Why?
  - Accuracy of the evaluated ND is dependent on the experimental data and their associated covariances (not just used to provide **bounds** to the values but also provide **weights** to the individual data sets).
  - The EXFOR database are often not complete and are missing important information to establish the **rigor/precision** of the experiment.
  - Oftentimes, uncertainties are **under reported** and **lack consistency** between different measurements by different groups and even same groups at different time period/facilities.



Template Uncertainty Method contd..

- How?
  - Templates are tailored for different reactions, measurement methods, energy ranges, and other relevant features.
  - For most cases, recommended uncertainty ranges are provided in relative % of the cross section. Sometimes they may be relative to other parameters.
  - Where the uncertainty needs to be propagated to the cross-section, other information may be required. For example, for (n,tot), the relationship between the yield and cross-section is not multiplicative. Therefore, propagation of background uncertainty requires knowledge of the sensitivities for proper error propagation.
  - Correlation for specific sources of uncertainties are recommended based on underlying physics and experiment information. Covariance matrices associated to each uncertainty source is constructed with this information.

Experimental Uncertainty Quantification (n,el)

- Different recommendations for TOF/mono-energetic sources.
- Much longer list of uncertainty recommendations based on the following sources.

Unc. source	Cor(Exp_i, Exp_i)	Cor(Exp_i, Exp_j) $i \neq j$
Timing-spread	From TOF $\rightarrow E_{out}$ transformation	≠0 for same facility/detector
Neutron-production target	Full	≠0 for same facility
Neutron-flux monitoring	Gaussian	≠0 for same facility/detector
Sample	Full	≠0 for similar target/methods
Geometric effects	Full	≠0 for same facility
Attenuation & multiple scatt.	Gaussian	Facility/methods dependent
Standards & references	From libraries	From libraries
Detector efficiency (neutrons)	Gaussian	Depends on efficiency determination
Detector efficiency (γ rays)	Full	Depends on efficiency determination
Extracting yields	Gaussian	≠0 for same facility/detector

Experimental Uncertainty Quantification (n,el) contd.

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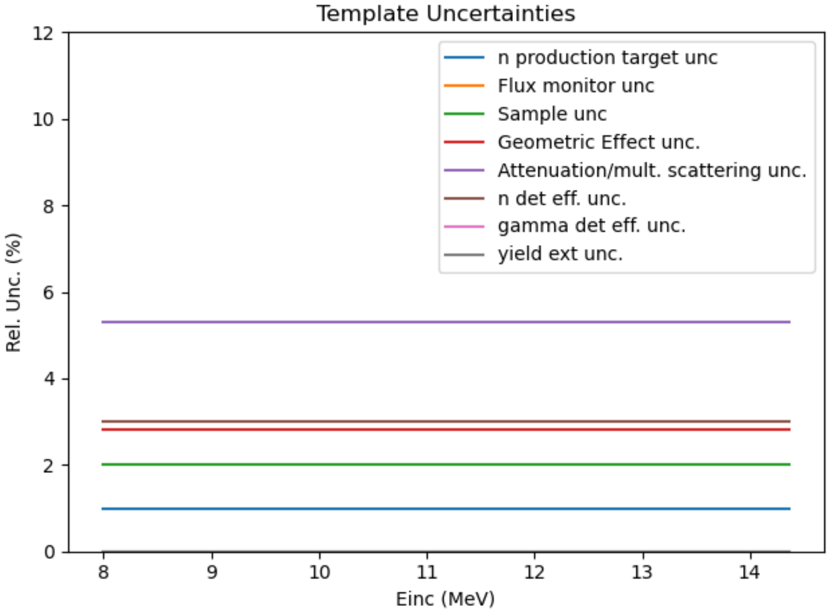
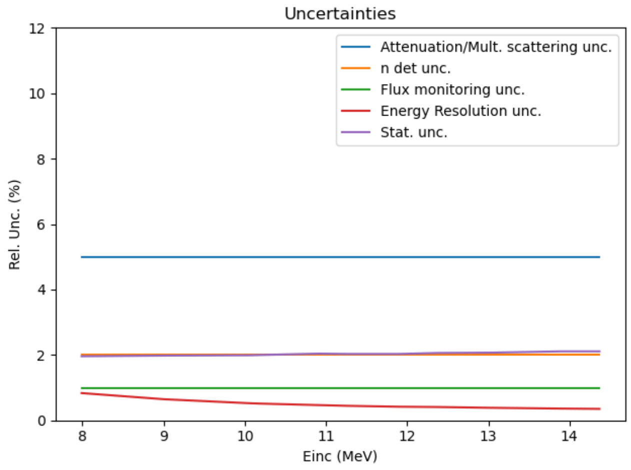


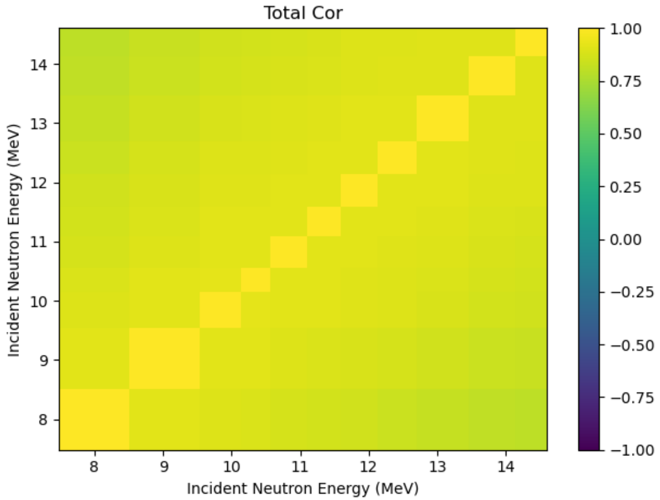
Rough ranges of different types of uncertainties from template based on Schmidt1996 data

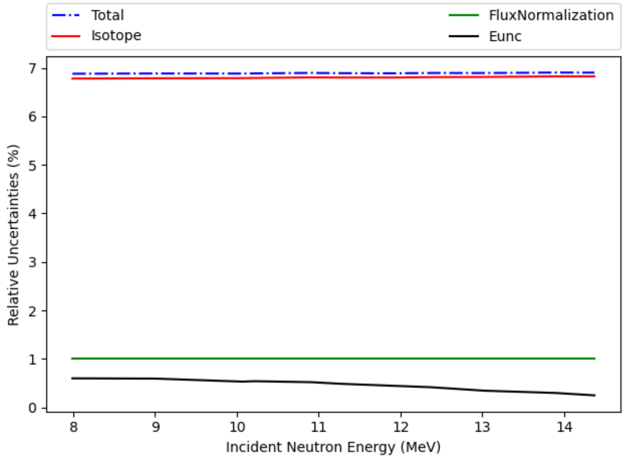
Not all available data could be accepted

Identifier	Energy Range (MeV)	Accepted/Rejected	Comments
n,tot			
Foster1971	2.384-14.859	Accepted	
Marshak1975	0.0014-0.1008	Rejected	Too low in energy to be relevant and not even statistical uncertainties are provided
Pineo1974	0.01452-0.627	Rejected	Too low in energy to be relevant and very high energy uncertainties
Rohr1967	0.02-0.221	Rejected	Too low in energy to be relevant
Rohr1996	0.25-19.979	Accepted	
Sorriaux1965	2.623-2.833	Accepted	
Thibault1967	2.7	Rejected	No information provided, not even areal density
Koester1988	0.143-2.1	Rejected	No identification of different source of uncertainties, not enough information to apply template
n,el			
Schmidt1996	2.99-14.4	Accepted	Although no documentation is available, few sources of uncertainty were identified in EXFOR
Harith1976	3.4	Accepted	Although no documentation is available, few sources of uncertainty were identified in EXFOR
Brandenberger1975	1.46	Rejected	No documentation; only stat unc and energy resolution available in EXFOR
Cabe1972	0.55-1.18	Rejected	No documentation; only stat unc and energy resolution available in EXFOR
Towle1965	1.61-2.35	Rejected	No documentation; only stat unc and energy resolution available in EXFOR

Example (n,el) - Schmidt1996







- Uncertainties from papers/EXFOR entries replace the template values where applicable (top left).
- Total covariance matrix (top right) is constructed from the sum of individual covariance matrices associated with each uncertainty source.
- UQed uncertainties and covariances, along with their features, are saved in .json format files.