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Title: Validating Evaluated Uncertainties of the Neutron-induced Fission Cross-sections by the Neutron Standards Data Project in ENDF/B-VIII.0 and Summarizing the  $^{239}\text{Pu}$  PFNS Evaluation of ENDF/B-VIII.0

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# Validating Evaluated Uncertainties of the Neutron-induced Fission Cross- sections by the Neutron Standards Data Project in ENDF/B-VIII.0 and Summarizing the $^{239}\text{Pu}$ PFNS Evaluation of ENDF/B-VIII.0

Denise Neudecker

WPEC, SG44

May 14-16, 2018

# Abstract

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The  $^{239}\text{Pu}$ ,  $^{238}\text{U}$  and  $^{235}\text{U}$  neutron-induced fission cross-sections and associated uncertainties in ENDF/B-VIII.0 [1] were provided by the “Neutron Standards Data” [2] project coordinated by the IAEA. The evaluated uncertainties increased in some energy ranges by a factor of 2 or more leading to significantly increased uncertainties on the criticality of specific critical assemblies [3]. This talk will highlight reasons why this increase of uncertainty is justified. The talk will also introduce the “Physical Uncertainty Boundary” [4] method which has been used to validate the size of these fission cross-section uncertainties independently.

This talk will cover as a second topic the evaluation of the  $^{239}\text{Pu}$  prompt fission neutron spectrum (PFNS) which is considered in ENDF/B-VIII.0.

[1] D.A. Brown et al., Nuclear Data Sheets Vol. 148, p. 1 (2018).

[2] A.D. Carlson et al., Nuclear Data Sheets Vol. 148, p. 143 (2018).

[3] M.B. Chadwick et al., Nuclear Data Sheets Vol. 148, p. 189 (2018).

[4] D.E. Vaughan et al., Los Alamos National Laboratory Report LA-UR-14-20441 (2014).

# Part 1: Validating Evaluated Uncertainties of the $^{239}\text{Pu}(n,f)$ Cross- Sections by the Neutron Standards Data Project in ENDF/B-VIII.0

Denise Neudecker

Thanks to: B. Hejnal, F. Tovesson, D.L. Smith, M.C. White, D. Vaughan, R. Capote, TPC collaboration (K. Schmitt, N. Bowden, L. Snyder, R. Casperson, N. Walsh, S. Sangiorgio, W. Younes)

# Validating increased evaluated uncertainties of the $^{239}\text{Pu}(n,f)$ cs in ENDF/B-VIII.0

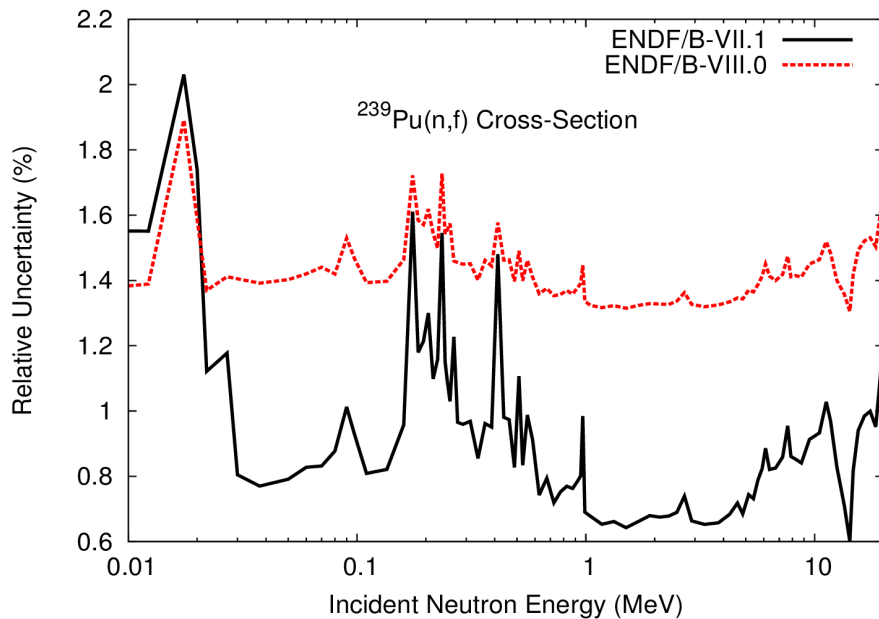
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- **Why should we validate increased  $^{239}\text{Pu}(n,f)$  cs uncertainties?**
- **Are there good reasons to increase the  $^{239}\text{Pu}(n,f)$  cs uncertainties from ENDF/B-VII.1 to ENDF/B-VIII.0?**
- **How can we validate evaluated  $^{239}\text{Pu}(n,f)$  cs uncertainties in ENDF/B-VIII.0?**

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# Why should we validate increased $^{239}\text{Pu}(n,f)$ cs uncertainties?

# $^{239}\text{Pu}(n,f)$ cross-section unc. were increased for ENDF/B-VIII.0 by expert judgment

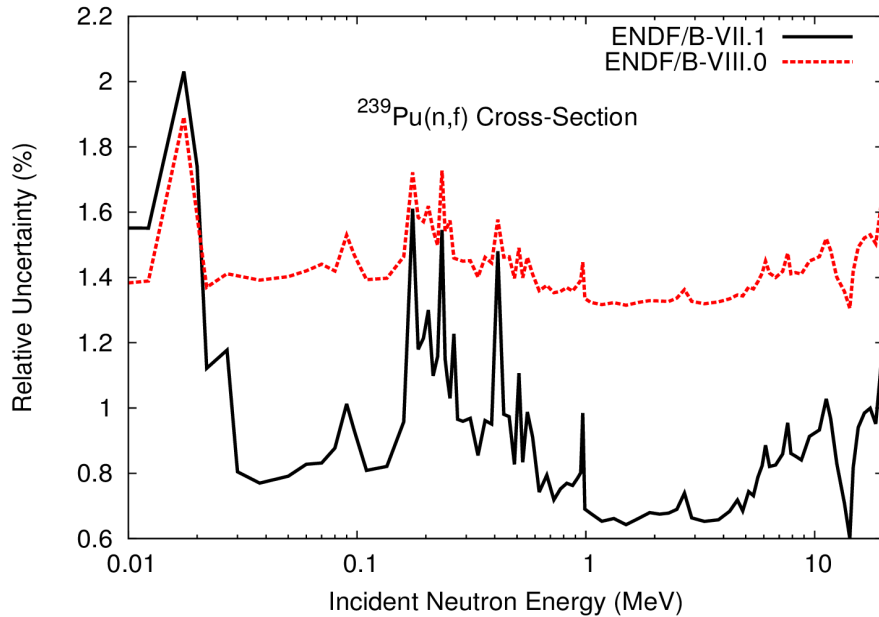


$^{239}\text{Pu}(n,f)$  VII.1 unc. were considered to be unrealistically small. Analysis of unknown systematic unc. by the standards evaluation committee (A. Carlson et al., NDS (2018)) led to increased unc.

$^{239}\text{Pu}(n,f)$  cs strongly impacts  $k_{\text{eff}}$  of Pu-assemblies. Jezebel  $k_{\text{eff}}$  unc. due to (n,f) cs increased from 331 pcm to 903 pcm.



# $^{239}\text{Pu}(n,f)$ cross-section unc. were increased for ENDF/B-VIII.0 by expert judgment



$^{239}\text{Pu}(n,f)$  VII.1 unc. were considered to be unrealistically small. Analysis of unknown systematic unc. by the standards evaluation committee (A. Carlson et al., NDS (2018)) led to increased unc.  $^{239}\text{Pu}(n,f)$  strongly impacts  $k_{\text{eff}}$  of Pu-assemblies.

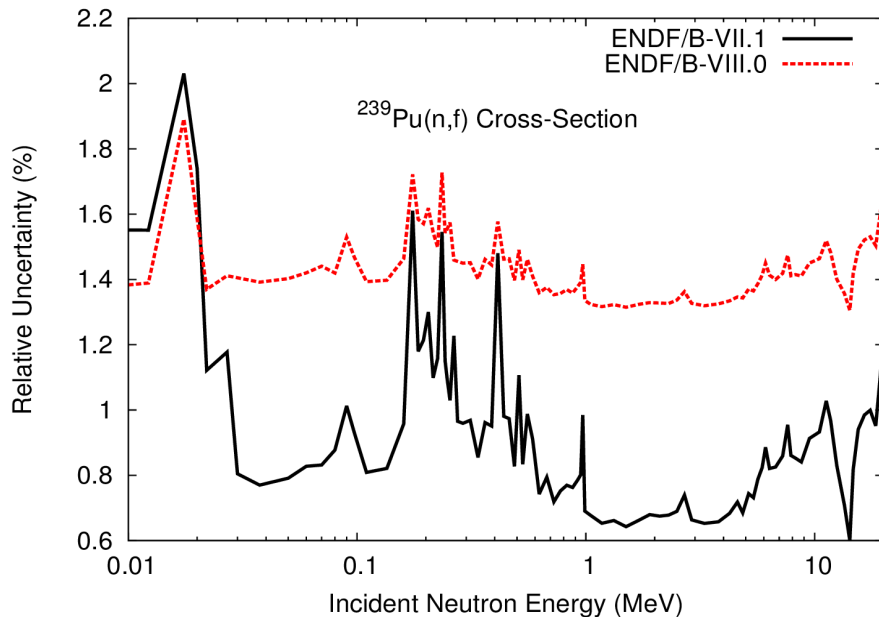
Unc. are underestimated because:

- Unrecognized unc. across many data sets due to using same methods.
- Missing cross-correlations between experimental data.
- Missing uncertainty sources for single experimental data sets.

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**Are there good reasons to  
increase the  $^{239}\text{Pu}(n,f)$  cs  
uncertainties from ENDF/B-  
VII.1 to ENDF/B-VIII.0?**

## Example 2: $^{239}\text{Pu}(n,f)$ cross-section unc. were increased for ENDF/B-VIII.0 by expert judgment



$^{239}\text{Pu}(n,f)$  VII.1 unc. were considered to be unrealistically small. Analysis of unknown systematic unc. by the standards evaluation committee (A. Carlson et al., NDS (2018)) led to increased unc.  $^{239}\text{Pu}(n,f)$  strongly impacts  $k_{\text{eff}}$  of Pu-assemblies.

Unc. are underestimated because:

- Unrecognized unc. across many data sets due to using same methods.
- Missing cross-correlations between experimental data.
- Missing uncertainty sources for single experimental data sets.

We investigate those via a template.

# A template of unc. typically encountered in fission cross-section measurements (LA-UR-17-29963):

Unc. Source	Typical range	Correlations	Cor(Exp <sub>1</sub> ,Exp <sub>2</sub> )
Sample Mass	> 1%	Full	Possible (same sample)
Counting Statistics	Sample-dependent	Diagonal	0
Attenuation	0.02-2%	Gaussian	Likely
Detector Efficiency	0-0.3%, 1-2%	Full < 10 MeV	Likely, 0.5-1.0
FF Angular Distrib.	~0.1%	Gaussian	Likely, 0.75-1.0
Background	0.2 - >10%	Gaussian	Possible
Energy Unc.	1%, 1-2 ns	Arises from conv.	Technique-dependent
Neutron Flux	0%, >1%	Full-0.5	Technique-dependent
Multiple Scattering	0.2-1%	Gaussian	0.5-0.75
Impurit. in Sample	Sample-dependent	1.0-0.9	0.5-0.75
Dead Time	>0.1%	Full	0

# The template distinguishes between different measurement types.

Unc. Source	Absolute	Clean Ratio	Indirect Ratio
Sample Mass	> 1%	Both Samples	Both samples
Counting Statistics	Sample-dependent	Both, combined	Both samples
Attenuation	0.2-2%	0.02-0.2%	0.2-2%
Detector Efficiency	1-2%	0-0.3%	1-2%, 0.5-1%
FF Angular Distrib.	~0.1%	Less than for abs.	~0.1%
Background	0.2 - >10%	0.2 - >10%	0.2 - >10%
Energy Unc.	1%, 1-2 ns	Combined	Both detectors
Neutron Flux	>1%	Cancels or small	Cancels or small
Multiple Scattering	0.2-1%	Reduced for abs.	0.2-1%
Impurit. in Sample	Sample-dependent	Both samples	Both samples
Dead Time	>0.1%	Both, combined	Both detectors

# This template can help evaluators and experimentalists estimate experimental unc.

- Templates were, e.g., developed for providing EXFOR data and uncertainties in the resonance region in F. Gunsing et al., INDC(NDS)-0647 (2013).
- Can provide guidelines for experimentalists **what uncertainties need to be provided for an evaluation.**
- Helps evaluators **pinpoint cross-correlations between other experiments** if the same template is used consistently.
- Helps evaluators **pinpoint missing experimental unc. of single experimental data sets.**

Applied that to data in the GMA database.

# Case 1, the absolute $^{239}\text{Pu}(n,f)/^{235}\text{U}(n,f)$ exp. with lowest unc. in the GMA database

Data Set	Data Type	Min $\delta$	Max $\delta$	Min $E$	Max $E$	EXFOR #
611	absolute	1.0	1.0	1.45E+01	1.45E+01	
644	absolute	2.0	2.0	1.45E+01	1.45E+01	30634
615	absolute	2.1	2.1	5.00E+00	5.00E+00	
1038	absolute	2.3	7.7	1.00E+00	5.50E-00	30670
640	absolute	2.4	3.1	1.50E-01	9.60E-01	10314
620	absolute	2.8	6.6	3.00E-02	9.80E-01	20567

Sample mass unc. should be ~1.5% questionably small!!!

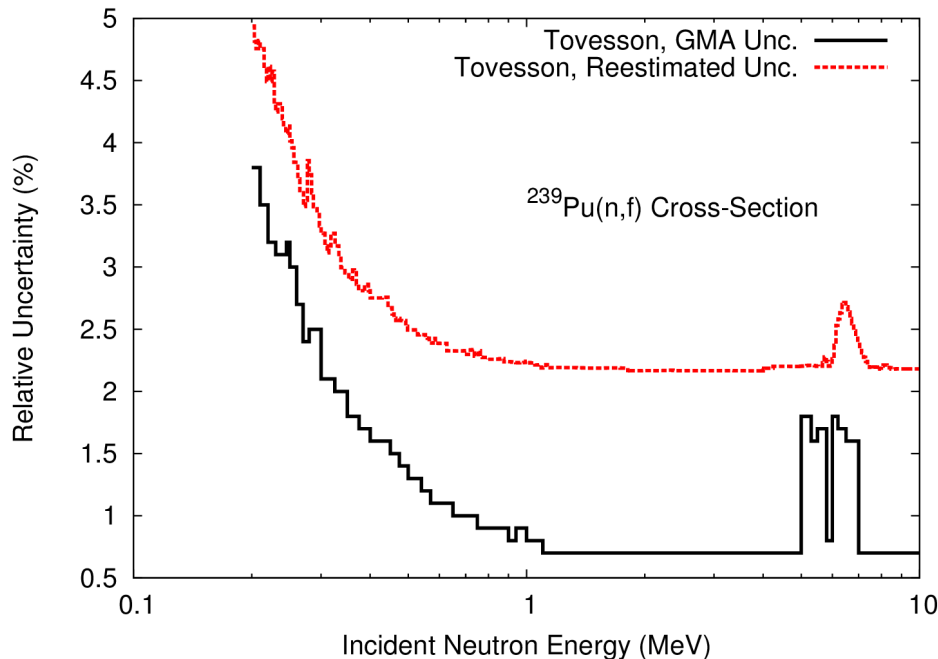
8002	ratio absolute $^{235}\text{U}(n,f)$	0.7	3.8	2.00E-01	1.30E+01	14271
602	ratio absolute $^{239}\text{U}(n,f)$	0.8	6.8	2.53E-08	1.00E-01	
654	ratio absolute $^{235}\text{U}(n,f)$	1.0	5.7	2.40E-02	7.50E+00	
685	ratio absolute $^{235}\text{U}(n,f)$	1.1	1.1	1.45E+01	1.45E-01	
653	ratio absolute $^{235}\text{U}(n,f)$	1.2	6.9	1.20E-01	7.00E+00	40824
1014	ratio absolute $^{235}\text{U}(n,f)$	1.3	1.6	8.50E-01	6.00E+01	13801
600	ratio absolute $^{235}\text{U}(n,f)$	1.7	27.4	8.50E-04	3.00E+01	10562
605	ratio absolute $^{235}\text{U}(n,f)$	1.7	15.3	5.50E-03	1.00E+00	20363
608	ratio absolute $^{235}\text{U}(n,f)$	2.0	12.6	4.50E-02	5.00E-01	21463
609	ratio absolute $^{235}\text{U}(n,f)$	2.0	2.1	1.00E+00	1.40E+01	21195
631	ratio absolute $^{235}\text{U}(n,f)$	2.1	2.1	2.53E-08	1.50E-01	
1012	ratio absolute $^{235}\text{U}(n,f)$	2.1	5.8	5.70E-01	2.00E+02	41455

630	ratio shape $^{10}\text{B}(n,\alpha)$	2.3	5.0	2.53E-08	1.50E-01	
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# E.g., a normalization uncertainty was overlooked for Tovesson et al. $^{239}\text{Pu}(n,f)/^{235}\text{U}(n,f)$



***This is the data set related to the  $^{239}\text{Pu}(n,f)$  cross-section in GMA with the lowest uncertainty!!!***

***→ We would need a measurement to the 0.7% level to strongly impact the GMA evaluation UNLESS WE UPDATE THE DATABASE!!!!!!!!!!!!!!!***



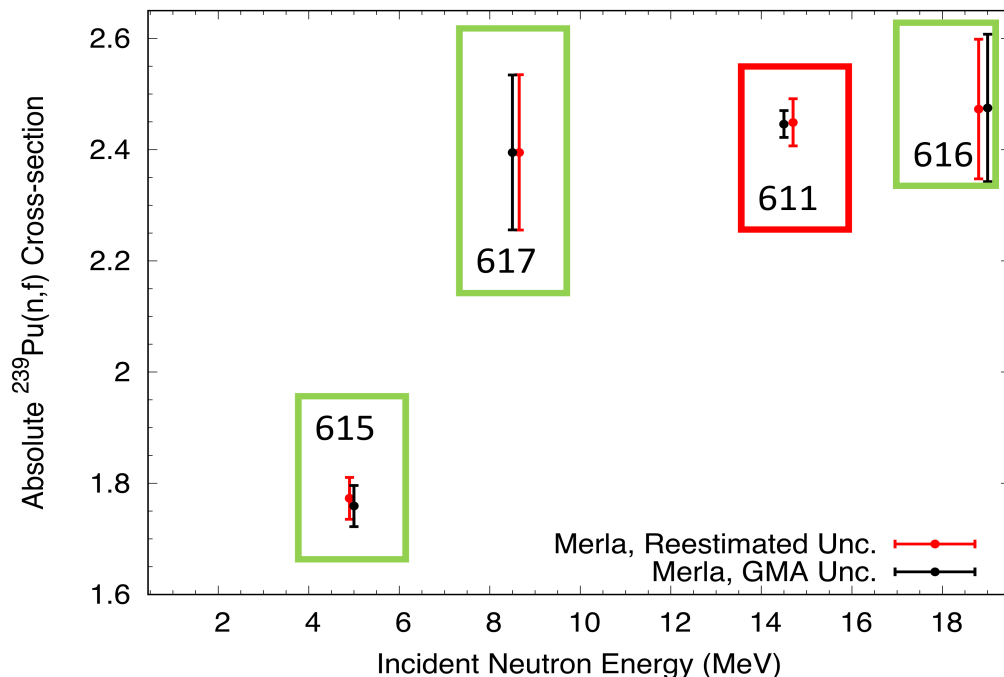
# Case 2: the absolute measurement with lowest unc. in GMA is strongly correlated with 3 other GMA exp.

This measurement is part of a series and correlated with 615-617.

Also, sample mass unc. Should be 1%, questionably small.

Data Set	Data Type	Min $\delta$	Max $\delta$	Min $E$	Max $E$	EXFOR #
611	absolute	1.0	1.0	1.45E+01	1.45E+01	
644	absolute	2.0	2.0	1.45E+01	1.45E+01	30634
615	absolute	2.1	2.1	5.00E+00	5.00E+00	
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620	absolute	2.8	6.6	3.00E-02	9.80E-01	20567
8002	ratio absolute $^{235}\text{U}(n,f)$	0.7	3.8	2.00E-01	1.30E+01	14271
602	ratio absolute $^{235}\text{U}(n,f)$	0.8	6.8	2.53E-08	1.00E-01	
654	ratio absolute $^{235}\text{U}(n,f)$	1.0	5.7	2.40E-02	7.50E+00	
685	ratio absolute $^{235}\text{U}(n,f)$	1.1	1.1	1.45E+01	1.45E-01	
653	ratio absolute $^{235}\text{U}(n,f)$	1.2	6.9	1.20E-01	7.00E+00	40824
1014	ratio absolute $^{235}\text{U}(n,f)$	1.3	1.6	8.50E-01	6.00E+01	13801
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609	ratio absolute $^{235}\text{U}(n,f)$	2.0	2.1	1.00E+00	1.40E+01	21195
631	ratio absolute $^{235}\text{U}(n,f)$	2.1	2.1	2.53E-08	1.50E-01	
1012	ratio absolute $^{235}\text{U}(n,f)$	2.1	5.8	5.70E-01	2.00E+02	41455
630	ratio shape $^{10}\text{B}(n,\alpha)$	2.3	5.0	2.53E-08	1.50E-01	

# Case 2: the absolute measurement with lowest unc. in GMA has too small unc. & is strongly correlated



611 GMA unc.: 1%

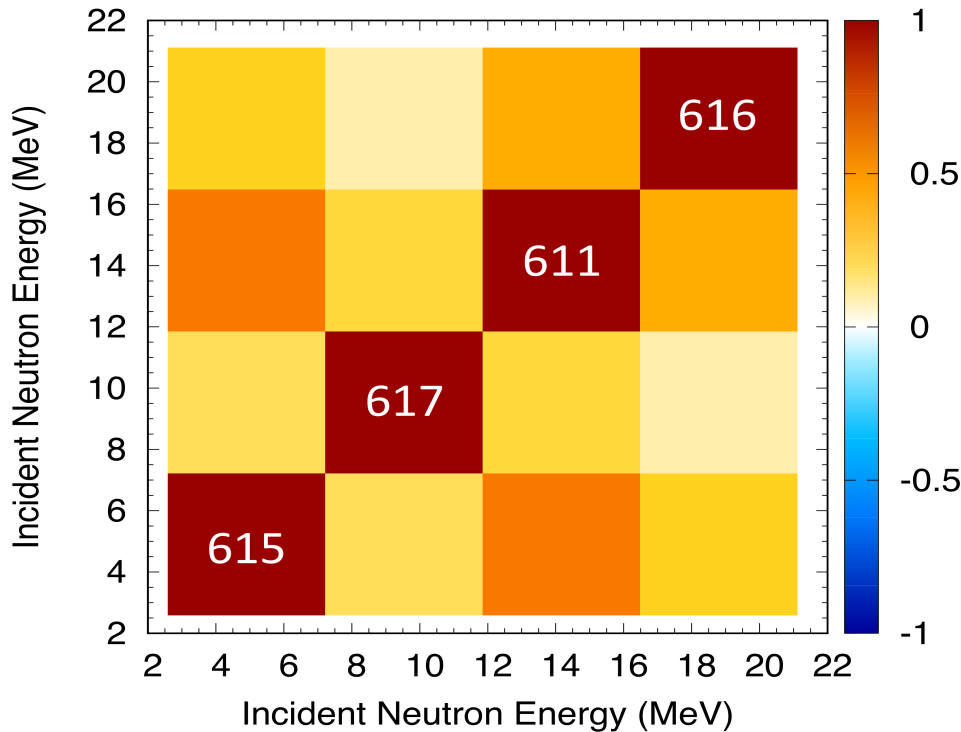
611 Reestimated unc.: **1.7%**

Sample mass unc. of 1% missing and background unc. of 0.5% missing.

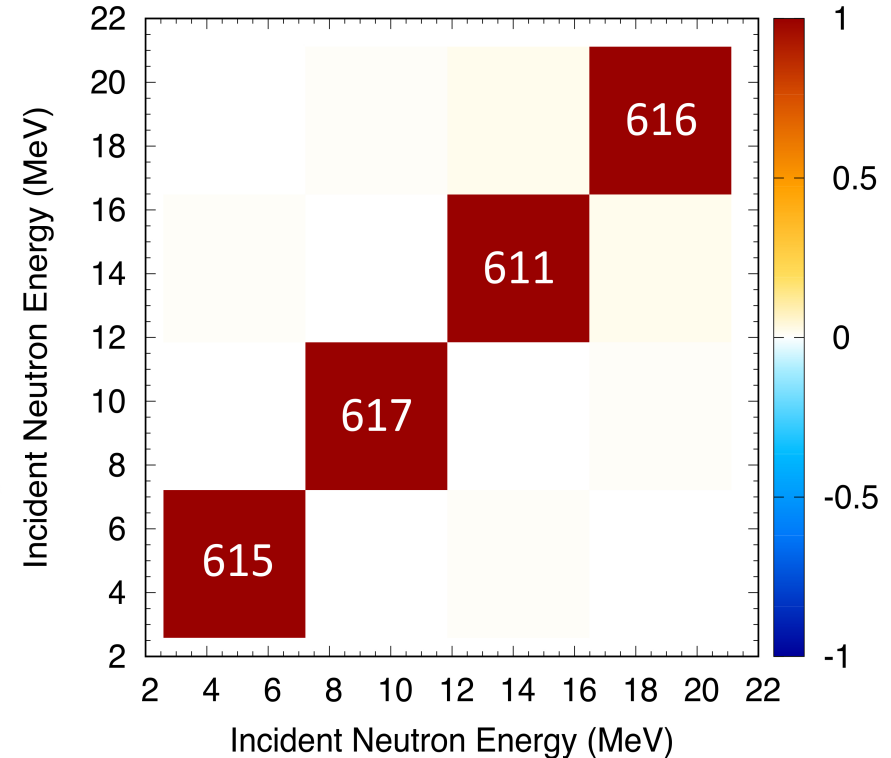
Cross-correlations arise because same sample was used, same detector, same multiple scattering correction, etc.

# Case 2: template helped to pin-point underestimated correlations in GMA

Reestimated Correlations



GMA Correlations



# These two cases of underestimated unc. are typical cases rather than exceptions!

GMA #	GMA unc.	Reestimated unc.
611	1.0	<b>1.7</b>
644	2.0	<b>2.2</b>
615	2.1	<b>2.4</b>
1038	2.3-7.7	2.3-7.7
640	2.4-3.1	<b>3.3-4.3</b>
620	2.8-6.6	<b>3.5-6.7</b>
622	2.8-7.0	<b>3.6-7.3</b>
619	2.9	<b>4.7</b>
621	2.9-3.2	<b>3.6-11.0</b>
623	3.2-4.1	<b>3.4-3.9</b>
612	3.8-4.7	<b>4.0-5.8</b>
672	4.9-5.4	<b>5.4-5.5</b>
616	5.4	5.1

GMA #	GMA unc.	Reestimated Unc.
617	5.8	5.8
628	5.9	<b>6.4</b>
657	9.3	9.3
521	2.3-4.8	<b>3.4-5.6</b>
589	2.9-3.9	<b>3.7-14.0</b>
671	4.3-25.8	<b>5.5-26.0</b>
8002	0.7-3.8	<b>2.2-4.9</b>
602	0.8-6.8	<b>1.5-6.9</b>
654+653	1.0-6.9	<b>1.8-75.5</b>
685	1.1	<b>2.0</b>
1014	1.3-1.6	<b>1.7-2.6</b>
536	0.7-6.5	<b>1.0-7.3</b>
1029	1.0-2.5	<b>2.5-3.5</b>

# If you order $^{239}\text{Pu}(n,f)$ according to lowest unc. & type of data, the order of reestimated unc. changes

GMA absolute data	Reestimated
611	611
644	644
<b>615</b>	<b>1038</b>
<b>1038</b>	<b>615</b>
640	640
<b>620</b>	<b>623</b>
<b>622</b>	<b>620</b>
<b>619</b>	<b>622</b>
621	621
<b>623</b>	<b>612</b>
<b>612</b>	<b>619</b>
<b>672</b>	<b>616</b>

GMA $^{239}\text{Pu}/^{235}\text{U}$	Reestimated
<b>8002</b>	<b>602</b>
<b>602</b>	<b>1014</b>
654+653	654+653
685	685
<b>1014</b>	<b>8002</b>

**Evaluated mean values and covariances are likely to change if new information is taken into account!!! An increased uncertainty compared to VII.1 is very likely!**

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# How can we validate evaluated $^{239}\text{Pu}(n,f)$ cs uncertainties in ENDF/B-VIII.0?

# Physical Uncertainty Boundaries (PUBs) methodology by D. Vaughan and D. Preston

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**PUBs methodology** (D.E. Vaughan, D.L. Preston, LANL Report LA-UR-14-20441 (2014)) was developed to **estimate the upper bounds** of a physical quantity **based on physics considerations** rather than optimization with physics models and experimental data. It was applied to estimate bounds of quantity of interests (QoI) of other physics areas.

**It is used here to validate the increased  $^{239}\text{Pu}(n,f)$  cs uncertainties. This methodology cannot give us mean values!!!**

# Using PUB methodology step-by-step

---

- 1) **Part** the QoI (here:  $^{239}\text{Pu}(n,f)$  cs) **into** its constituting independent **sub-processes**.
- 2) **Establish the dominant sub-processes**, i.e., those that contribute the most to the variability of the  $^{239}\text{Pu}(n,f)$  cs .
- 3) Answer: what are the **most extreme values** you could imagine **for the dominating sub-processes**? Or what is the most extreme variability on the  $^{239}\text{Pu}(n,f)$  cs you could imagine coming from the variability of the sub-process?
- 4) What is the **functional form** of the variability on the  $^{239}\text{Pu}(n,f)$  cs due to the dominant sub-processes?



# (1) $^{239}\text{Pu}(n,f)$ cs in VIII.0 is evaluated based on exp. data only → part an experiment into sub-processes

$$cs(E) = \frac{N(C(E) - C_b(E))\beta(E)\alpha(E)m(E)}{\epsilon(E)\varphi(E)d(E)} - \sum_i \zeta_i(E) \quad \text{with } \zeta_i = N_i cs_i(E)$$

N ... number of atoms in the sample

C ... total counts

$N_i$  ... number of atoms from impurity

$\varphi$  ... neutron flux

Measured separately

d ... dead time correction

m ... multiple scattering correction

$\beta$  ... attenuation correction

$\alpha$  ... fission fragment angular distribution correction

$CS_i$  ... cross section of contamination

Simulated or given by data

$\epsilon$  ... detector efficiency

$C_b$  ... background counts

Simulated and measured

## (2) From the template we establish which sub-processes contribute the most to the variability.

$$CS(E) = \frac{N(C(E) - C_b(E))\beta(E)\alpha(E)m(E)}{\epsilon(E)\varphi(E)d(E)} - \sum_i \zeta_i(E) \quad \text{with } \zeta_i = N_i CS_i(E)$$

**N ... number of atoms in the sample**

C ... total counts

$N_i$  ... number of atoms from impurity

**$\varphi$  ... neutron flux**

Measured separately

d ... dead time correction

**m ... multiple scattering correction**

**$\beta$  ... attenuation correction**

$\alpha$  ... fission fragment angular distribution correction

$CS_i$  ... cross section of contamination

Simulated or given by data

**$\epsilon$  ... detector efficiency**

**$C_b$  ... background counts**

Simulated and measured

### (3) I use the template to obtain extreme variability of $^{239}\text{Pu}(n,f)$ cs due to variability in sub-processes

Unc. Source	Typical range	Correlations	Cor(Exp <sub>1</sub> ,Exp <sub>2</sub> )
Sample Mass	> 1%	Full	Possible (same sample)
Counting Statistics	Sample-dependent	Diagonal	0
Attenuation	0.02-2%	Gaussian	Likely
Detector Efficiency	0-0.3%, 1-2%	Full < 10 MeV	Likely, 0.5-1.0
FF Angular Distrib.	~0.1%	Gaussian	Likely, 0.75-1.0
Background	0.2 - >10%	Gaussian	Possible
Energy Unc.	1%, 1-2 ns	Arises from conv.	Technique-dependent
Neutron Flux	0%, >1%	Full-0.5	Technique-dependent
Multiple Scattering	0.2-1%	Gaussian	0.5-0.75
Impurit. in Sample	Sample-dependent	1.0-0.9	0.5-0.75
Dead Time	>0.1%	Full	0

Well, actually these are not the most extreme uncertainties you can get on each sub-processes (you can always do something wrong in your experiments :-)) but a reasonable accuracy to which you can get each sub-processes with a standard measurement.

**We believe that it is hard to describe the sub-processes with better accuracy.**

## (4) What is the functional form of the sub-processes? A few examples.

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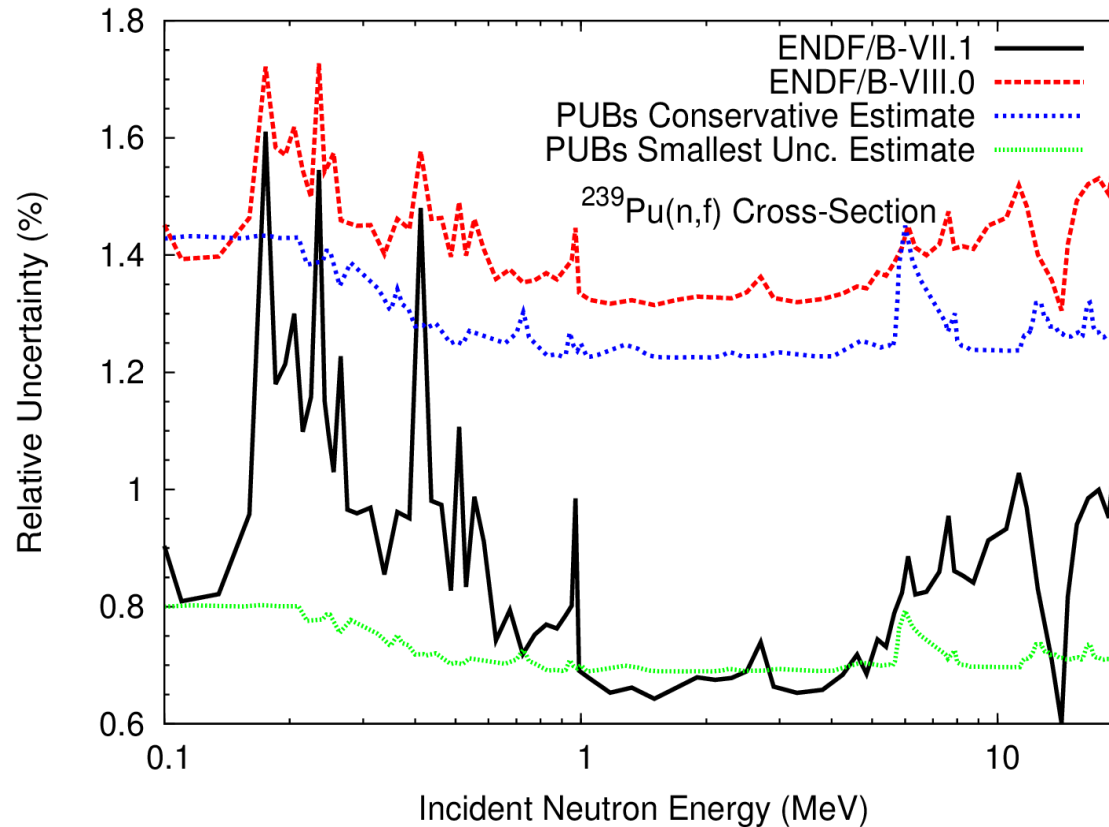
- $N$ : this is the same for the whole cross-section measurement, i.e., a linear coefficient of the cross-section.
- $\epsilon$ : for  $E < 10$  MeV, this is a constant factor, i.e., a linear coefficient of the cross-section. Then another functional form sets in.
- $C_b$ : defined by a functional form with few parameters + nuclear data used in a code. I assume a Gaussian kernel.

## (5) Total bounds are obtained by considering correlations between experiments.

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- Assess how unc. of each sub-process reduce if measured multiple times, i.e., are the uncertainties **correlated between experiments**? If “Yes”, how high is the correlation? How many experiments are considered?
- **Combine the resulting average uncertainties of each sub-process**
- ***We cannot assess those uncertainties which were overlooked in all experiments because they use very similar methods. So while a reasonable bound it might not be the upper bound.***

# (5) The conservative bound of PUBs is close to the ENDF/B-VIII.0 evaluated uncertainties.



# Conclusions:

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- **VIII.0  $^{239}\text{Pu}(n,f)$  cs unc.** were investigated and validated because they **increased by more than a factor of 2** in some energy range **impacting significantly  $k_{\text{eff}}$  unc.** of specific assemblies.
- **Are there good reasons** to increase the  $^{239}\text{Pu}(n,f)$  cs uncertainties from ENDF/B-VII.1 to ENDF/B-VIII.0? **YES! Uncertainties of single experimental data sets and correlations between different experiments are missing** for many data sets underlying the standards evaluation. **If the standards database is updated with this information, mean values and unc. will change likely.**
- $^{239}\text{Pu}(n,f)$  cs uncertainties in **ENDF/B-VIII.0** were **validated by PUBs** methodology. **VIII.0 unc. are a bit higher than a conservative PUBs estimate.**

# Part 2: Summarizing the $^{239}\text{Pu}$ PFNS Evaluation of ENDF/B-VIII.0

Denise Neudecker

Thanks to: P. Talou, T. Kawano, R. Capote, D.L. Smith, T. Taddeucci,  
R.C. Haight, M. Devlin, K. Kelly, J. Gomez, A.C. Kahler, M.C. White,  
M.E. Rising, J. O'Donnell, B. Kiedrowski, D.G. Madland



# The $^{239}\text{Pu}$ PFNS Evaluation of ENDF/B-VIII.0:

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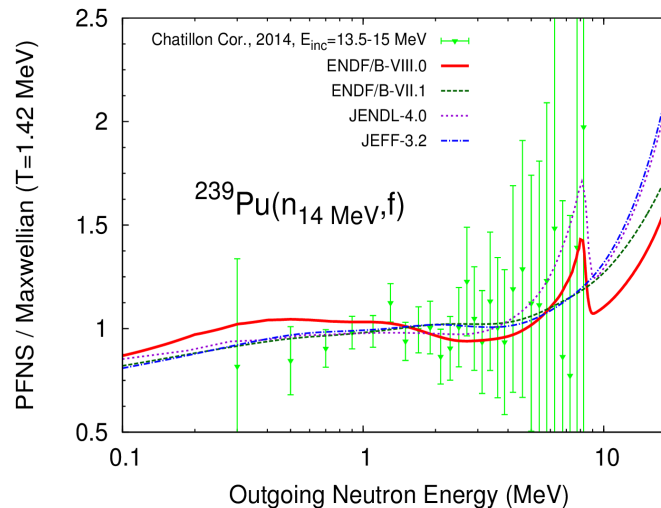
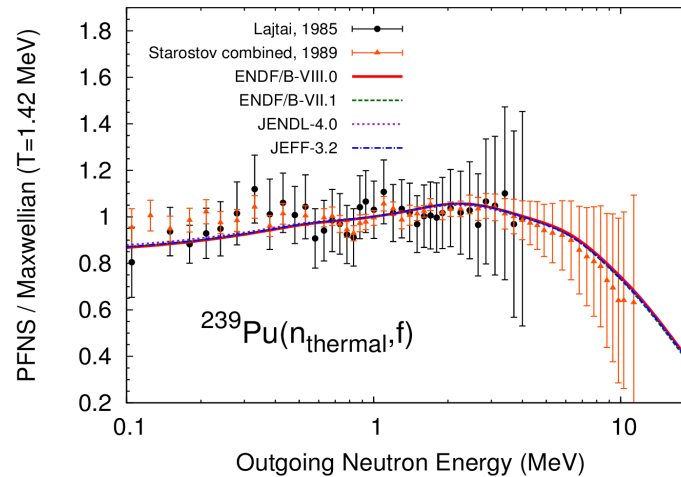
- Comparing ENDF/B-VII.1 and ENDF/B-VIII.0  $^{239}\text{Pu}(n,f)$  PFNS mean values and how they were evaluated.
- Comparing ENDF/B-VII.1 and ENDF/B-VIII.0  $^{239}\text{Pu}(n,f)$  PFNS covariances and how they were evaluated.
- What should we do better for the next evaluation?

# Comparing $^{239}\text{Pu}$ PFNS evaluated mean values

## ENDF/B-VII.1

Evaluated by D.G. Madland for ENDF/B-VII.0

**ENDF/B-VII.1 was carried over to maintain good agreement of benchmarks while waiting for new experimental data.**



## ENDF/B-VIII.0

Thermal: **VII.1** was slightly hardened to increase criticality benchmark performance

0.5-5 MeV: carried over from **VII.1**

> 5 MeV: **new evaluation** by D. Neudecker et al., NDS 148, 293 (2018).

# Comparing $^{239}\text{Pu}$ PFNS evaluated mean values

	<u>ENDF/B-VII.1</u>	<u>ENDF/B-VIII.0, <math>E_{inc} &gt; 5 \text{ MeV}</math></u>
Model	Original LAM as by D.G. Madland, NSE 81, 213 (1982), no pre-equilibrium component	Extended LAM (D. Neudecker et al., NIMA 791, 80 (2015).), exciton model for pre-equilibrium component (DN NDS 148.)
PFNS Exp.	Knitter, Staples et al.	Starostov, Boytsov, Nefedov et al., Knitter, Lestone et al., Lajtai et al., Chatillon et al.
Eval. Technique	LS for $E_{inc} < 6 \text{ MeV}$ , above grid-search minimization to fit model parameters	GLS

# Comparing $^{239}\text{Pu}$ PFNS evaluated covariances

## ENDF/B-VII.1

Evaluated by P. Talou et al., NSE 166, 254 (2010). Given for  $E_{\text{inc}}$  up to 0.5 MeV.

**The evaluated data and covariances were obtained independently but evaluated mean values agreed well.**

## ENDF/B-VIII.0

$E_{\text{inc}}$  up to 0.5 MeV: carried over from **VII.1** and **applied up to 5 MeV** as physics and consequently covariances are very similar.

**$E_{\text{inc}} > 5$  MeV: new evaluation** by D. Neudecker (NDS 148, NIMA). **Covariances were evaluated with mean values.**

# Comparing $^{239}\text{Pu}$ PFNS evaluated covariances

	<u>ENDF/B-VII.1</u>	<u>ENDF/B-VIII.0</u>
Model	Original LAM, <b>unc. for 4 model parameters</b> by PT NSE.	Extended LAM + multiple-chance fission, <b>unc. for ~22 model parameters</b> (DN NDS 148. & NIMA)
PFNS Exp.	<b>Simplified unc. estimate</b> for Knitter, Staples et al., Boytsov et al., Lajtai et al.	Starostov, Boytsov, Nefedov et al., Knitter, Lestone et al., Lajtai et al., Chatillon et al. → <b>detailed unc. estimate</b> in D. Neudecker et al., NDS 131, 289 (2016).
Eval. Technique	Kalman filter	GLS

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# What should we do better for the next evaluation?

# GLS was used for new VIII.0 and the Kalman filter was used for VII.1 covariances.

The **generalized least squares algorithm** combines **model (“M”)** and **experimental mean values (“x”)** and their associated covariances to evaluate mean values and covariances (“post”).

$$\underline{\phi}^{post} = \underline{\phi}^M + \mathbf{Cov}^{post} \mathbf{S}^+ (\mathbf{Cov}^x)^{-1} (\underline{\phi}^x - \mathbf{S} \underline{\phi}^M),$$





$$\mathbf{Cov}^{post} = \mathbf{Cov}^M - \mathbf{Cov}^M \mathbf{S}^+ (\mathbf{S} \mathbf{Cov}^M \mathbf{S}^+ + \mathbf{Cov}^x)^{-1} \mathbf{S} \mathbf{Cov}^M$$

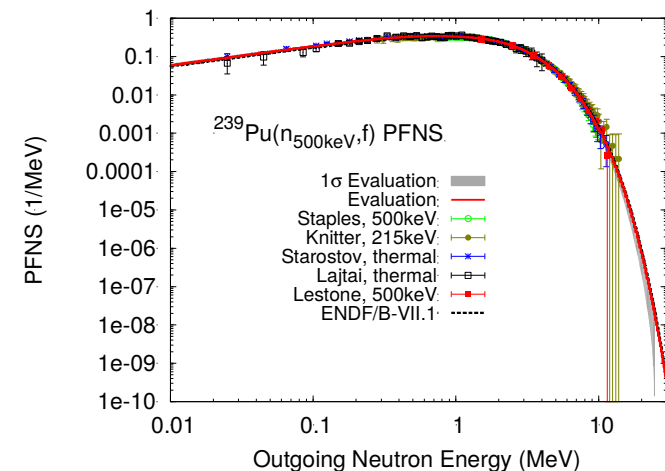
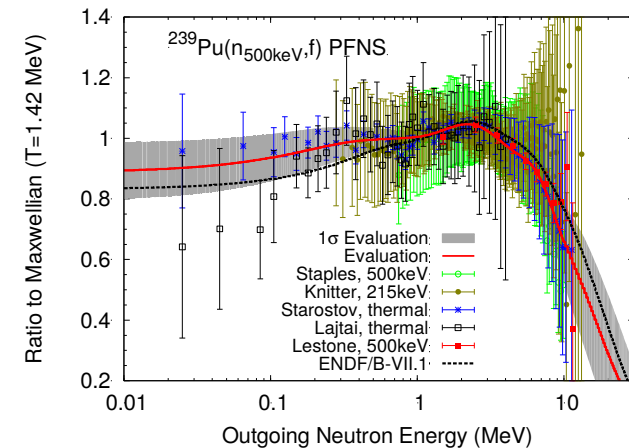
It **assumes that:**

- Experimental data and model values to be **normally distributed.**
- Linear relationship** between all observables.
- Non-discrepant data.**
- Data that **is less than ~30% uncertain.**
- Data that should **not cover many orders of magnitude.**

# Generalized least squares is not ideal for evaluating PFNS

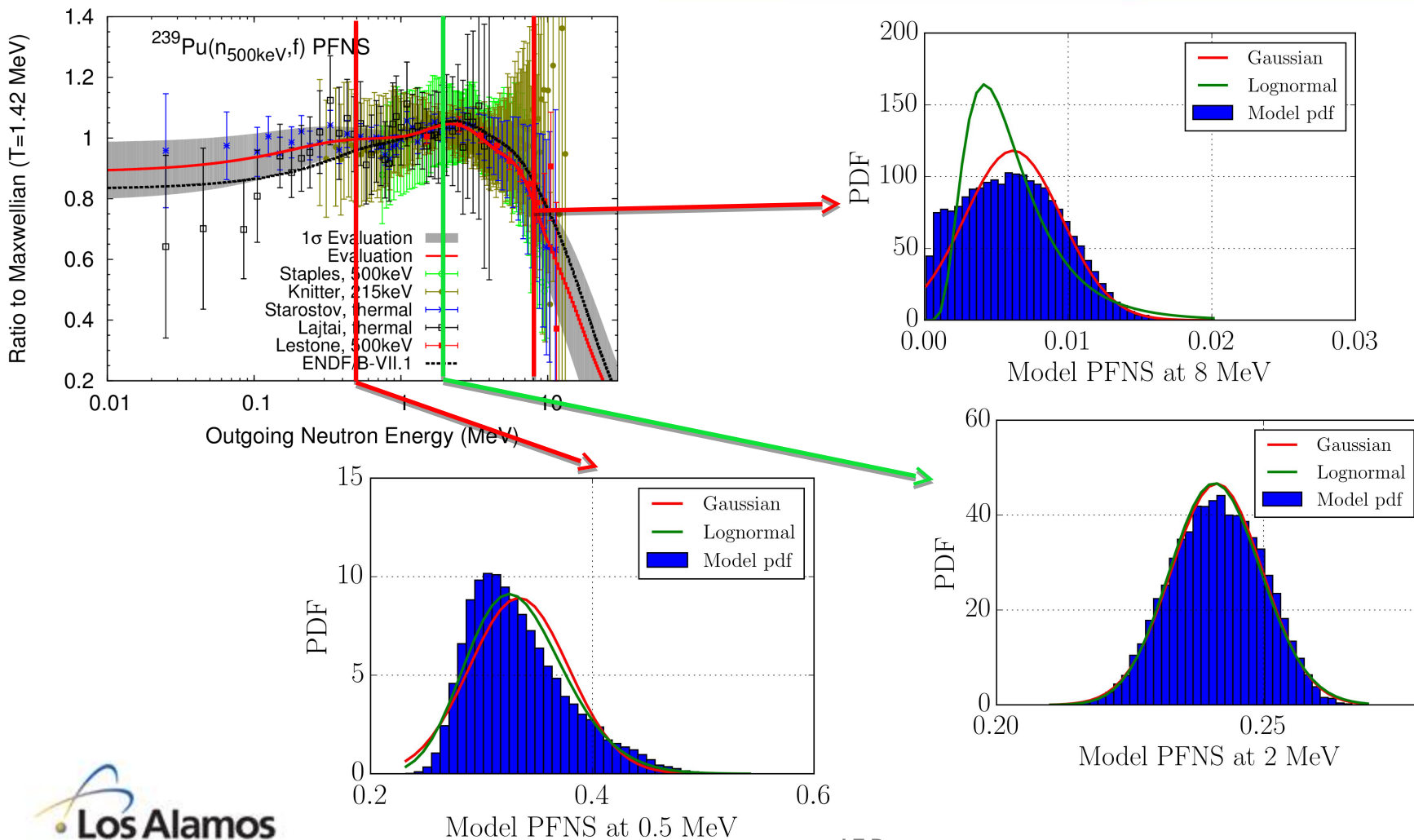
It requires:

- **Linear relationship** between all observables. + VIII.0 yes, VII.1 no
- **Non-discrepant data.** 
- Data that is **less than ~30% uncertain.** 
- Data that should **not cover many orders of magnitude.** 
- Experimental data and model values to be **normally distributed.** 

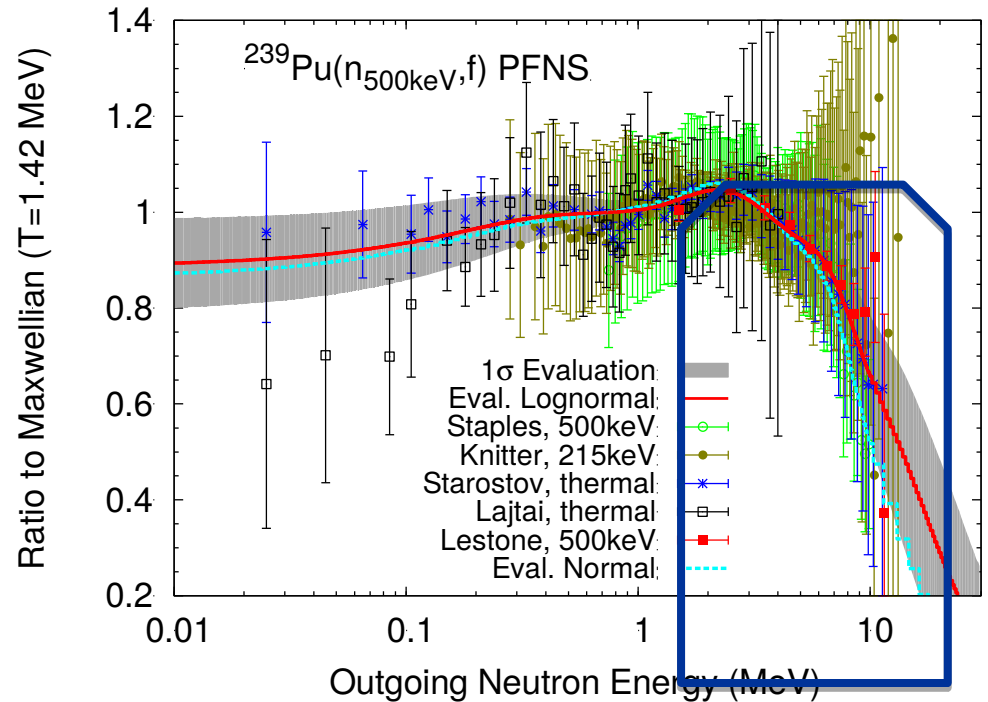
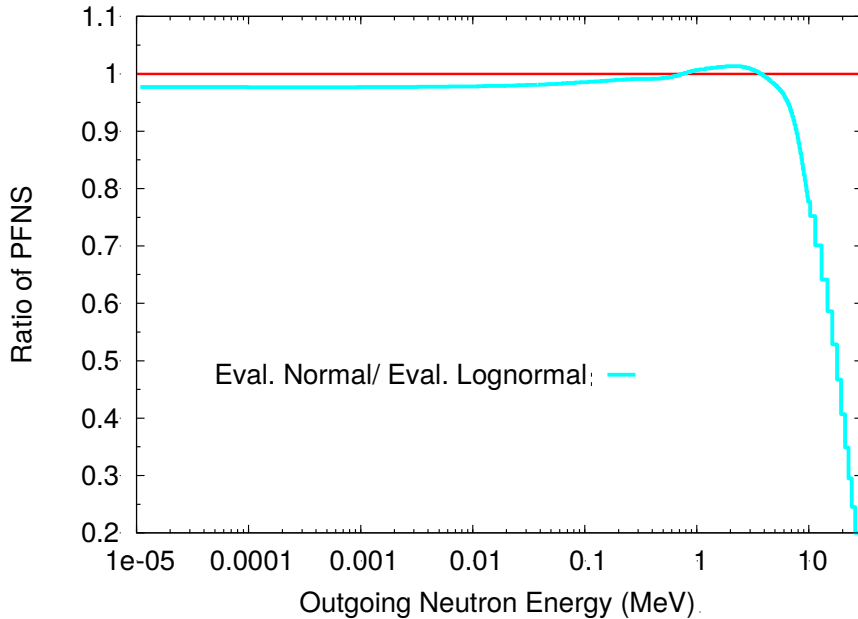




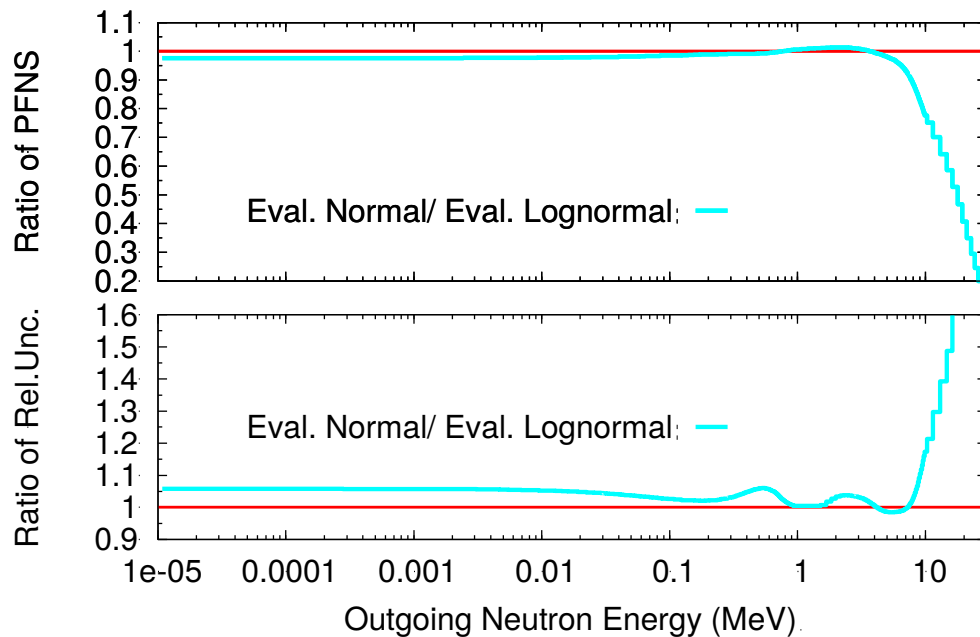
# Model predicted values are neither normally nor lognormally distributed ...



# ... and evaluating with GLS in PFNS or log space gives different evaluated results ...



# Evaluating with GLS in PFNS or log space impacts $k_{eff}$ results distinctly, $k_{eff}$ unc. only little.

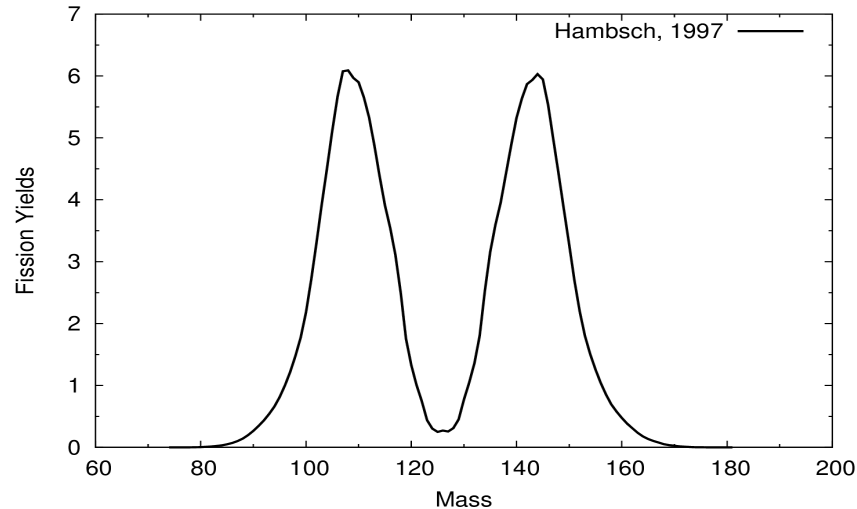
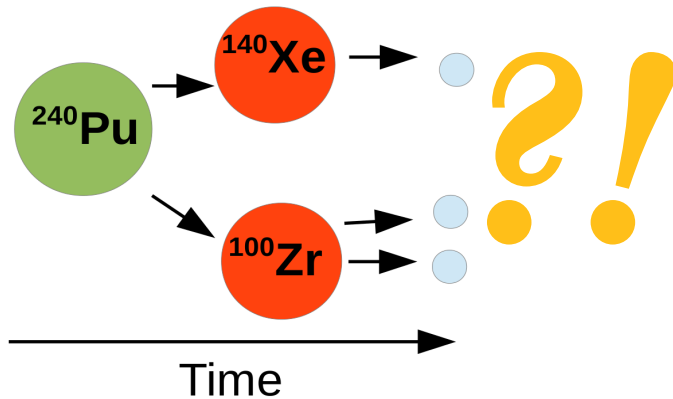


**Change in Jezebel  $k_{eff}$ :**  
**-89 pcm**

Increased Jezebel  $k_{eff}$   
unc. due to PFNS  
uncertainty:  
**+3.8%**

# Model development: switching to models which describes the fission process in more detail.

## First Chance Fission

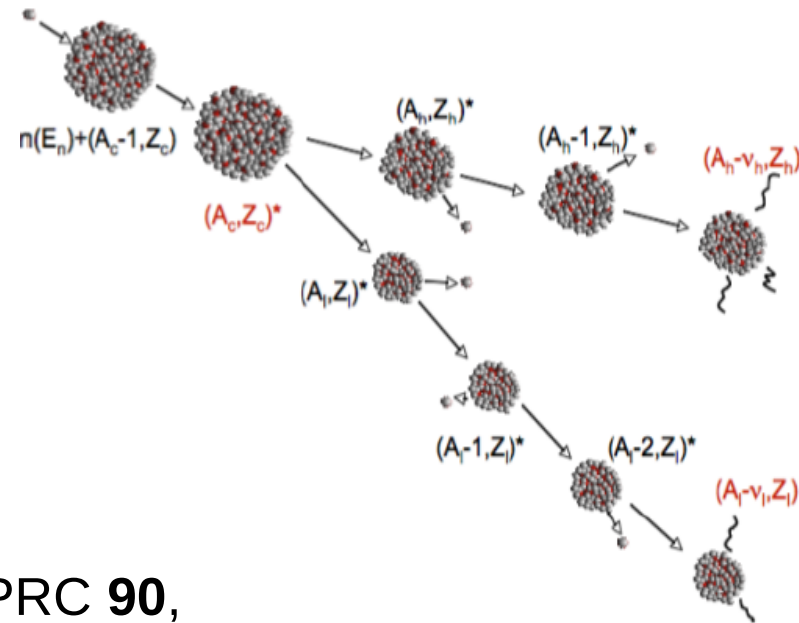


Original **LAM** assumes that neutrons are emitted from one average fission fragment pair and does not take into account the real distribution of fission fragments. This is just one of **many approximations**.

# Model development: predicting correlated fission observables based on more physics input.

**GGMF code** (Talou, I. Stetcu, T. Kawano) samples from initial distribution of fission fragments and follows each decay step via Hauser-Feshbach model.

Provide **predictions of several fission quantities** (PFNS,  $p(\nu)$ , PFGS, etc.) and several isotopes  
→ **MORE (measurable) INPUT QUANTITIES NEEDED.**



e.g.: I. Stetcu et al., PRC **90**, 024617 (2014).

# Summary

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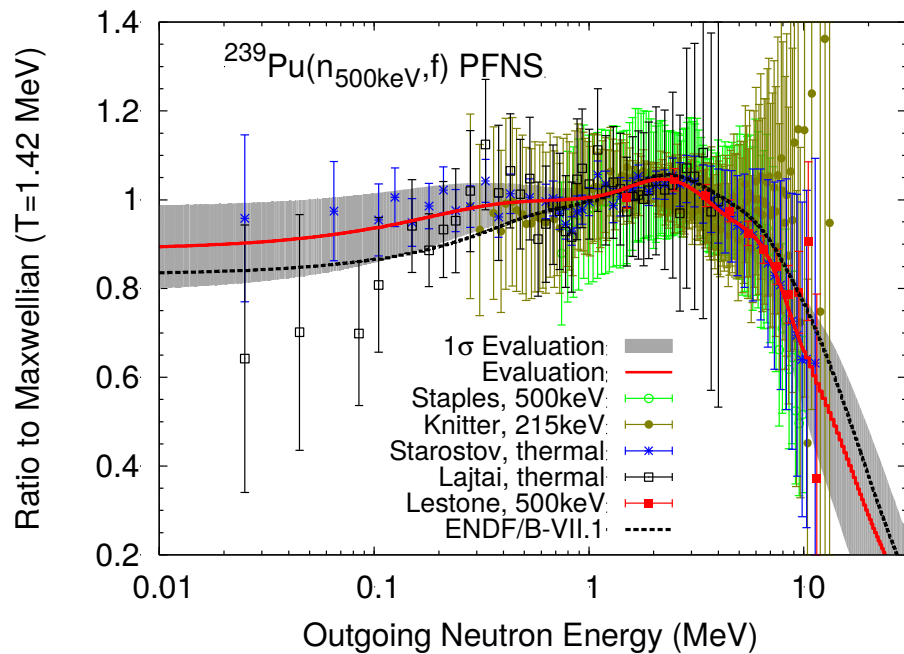
- **ENDF/B-VIII.0  $^{239}\text{Pu}(n,f)$  PFNS mean values are mostly carried over from VII.1 up to  $E_{\text{inc}} = 5$  MeV. Above a new evaluation was adopted including more experimental data sets and extended modeling.**
- **ENDF/B-VIII.0  $^{239}\text{Pu}(n,f)$  PFNS covariances were carried over from VII.1 up to  $E_{\text{inc}} = 5$  MeV. New files are given above. This covariances are based on a detailed analysis of experimental and mode uncertainties.**
- **The next evaluation will be likely based on a new physics model. Novel evaluation techniques should be studied.**

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# Backup

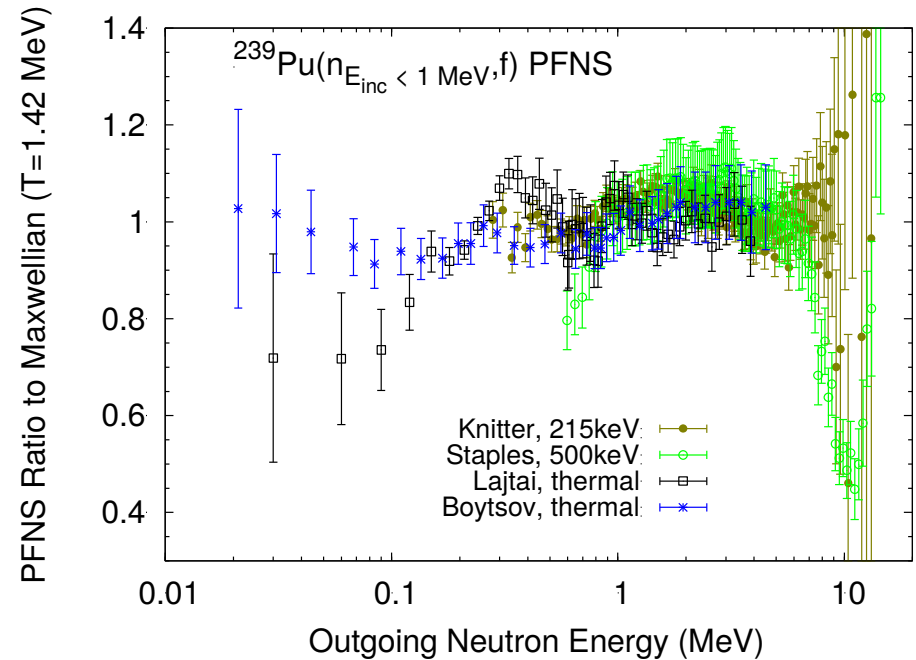
# Taking data blindly from our databases (which people do!) is not a good idea ...

## Detailed uncertainty estimate



Detailed analysis of data and uncertainties.

## Simplified uncertainty estimate

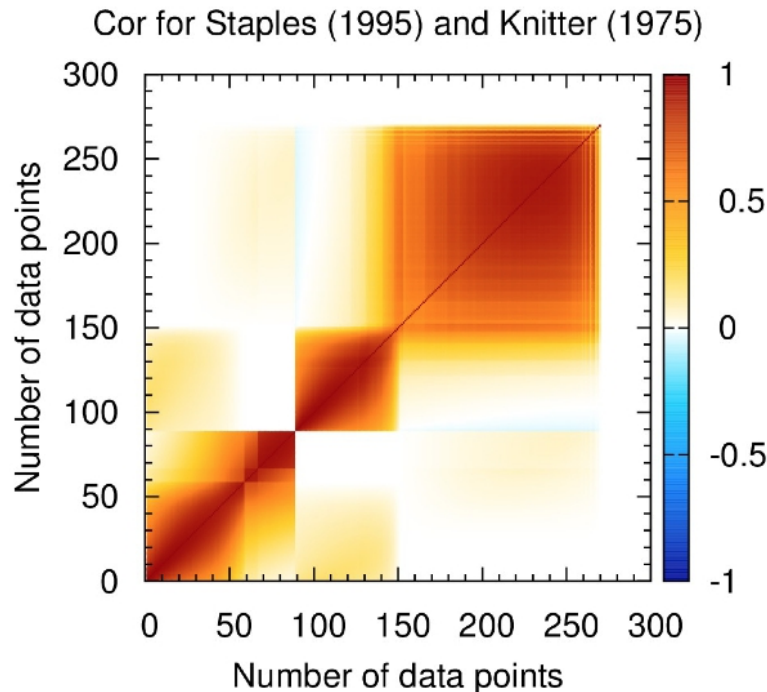


**Data and uncertainties taken as is from our databases discrepant!**



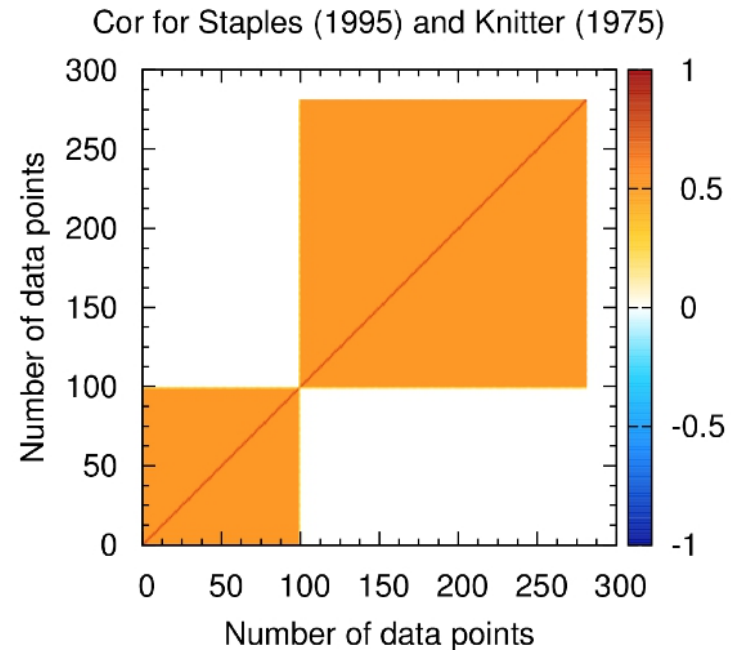
# Estimating detailed experimental uncertainties is time-intensive because ...

## Detailed uncertainty estimate



Recommended approach to estimate unc. was taken.

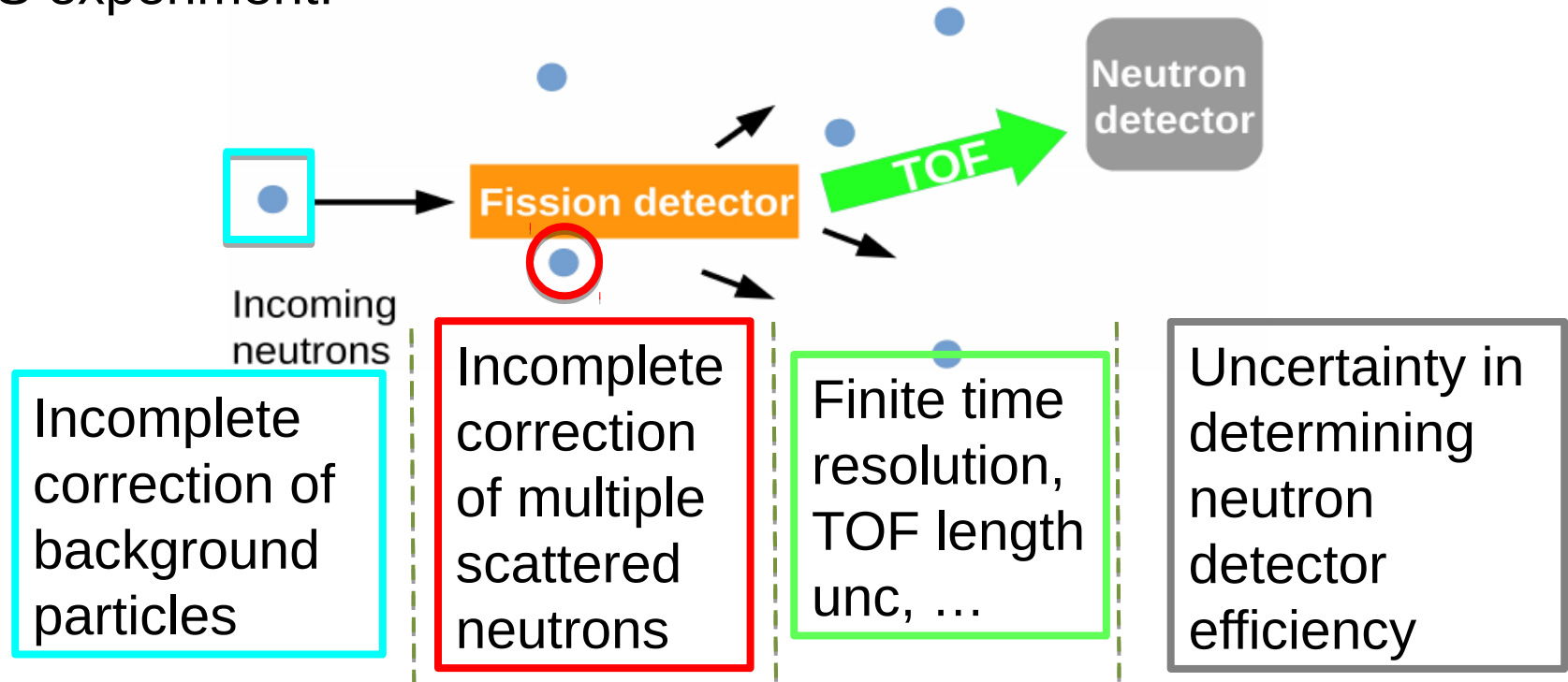
## Simplified uncertainty estimate



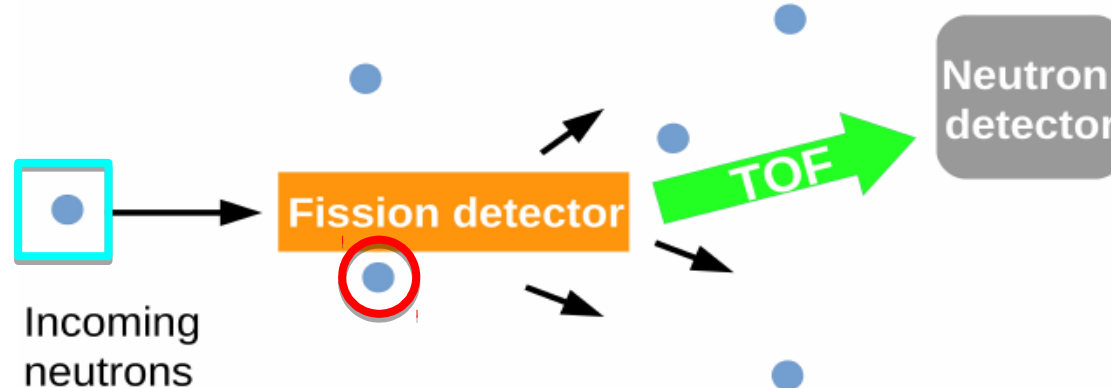
Total uncertainties extracted from EXFOR and correlations of same exp. are 0.5, otherwise 0.

# Detailed uncertainty estimate: First estimate covariances of partial uncertainties ...

Possible uncertainty sources of a PFNS experiment:



# ... then add up partial covariances.

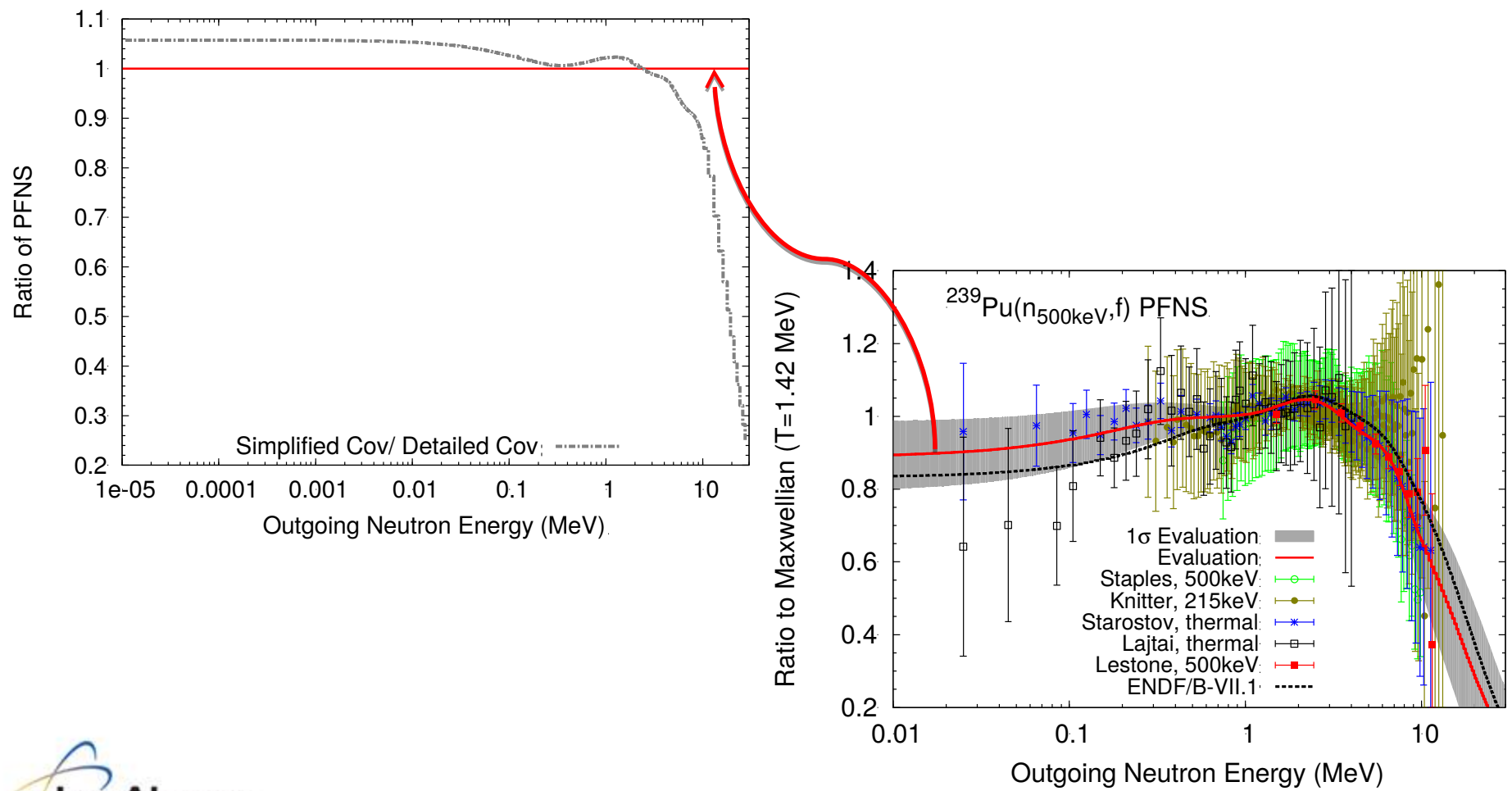


$$Cov^{exp} = Cov^{Count. Stat.} + Cov^{Backgd.} + Cov^{Mult. Scatt.} + Cov^{TOF} + Cov^{Det. Eff.} + \dots$$

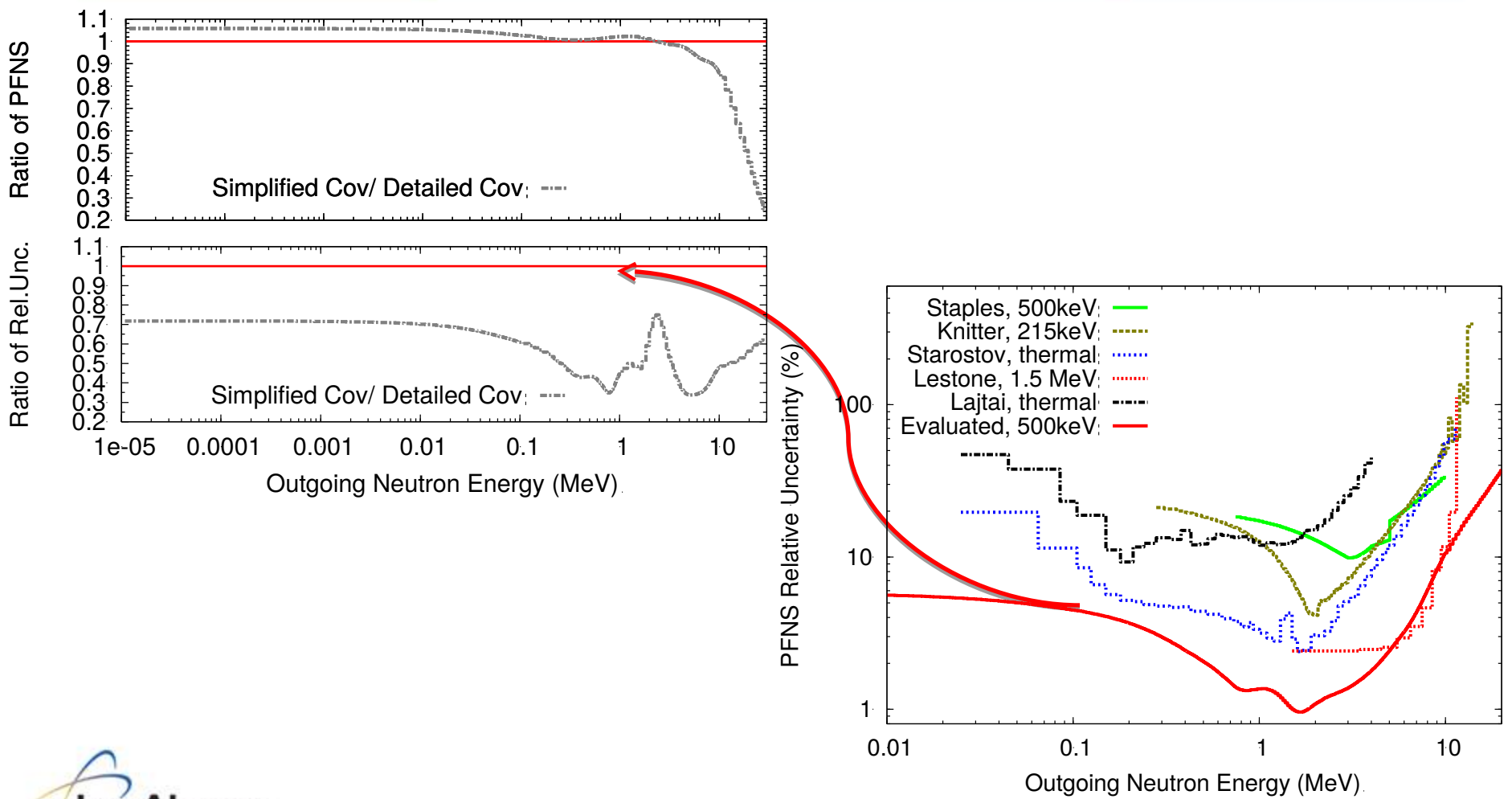
## Advantages:

- Same technique can be used to **estimate covariances between experiments** more transparently.
- Additional **uncertainties can be easily added.**

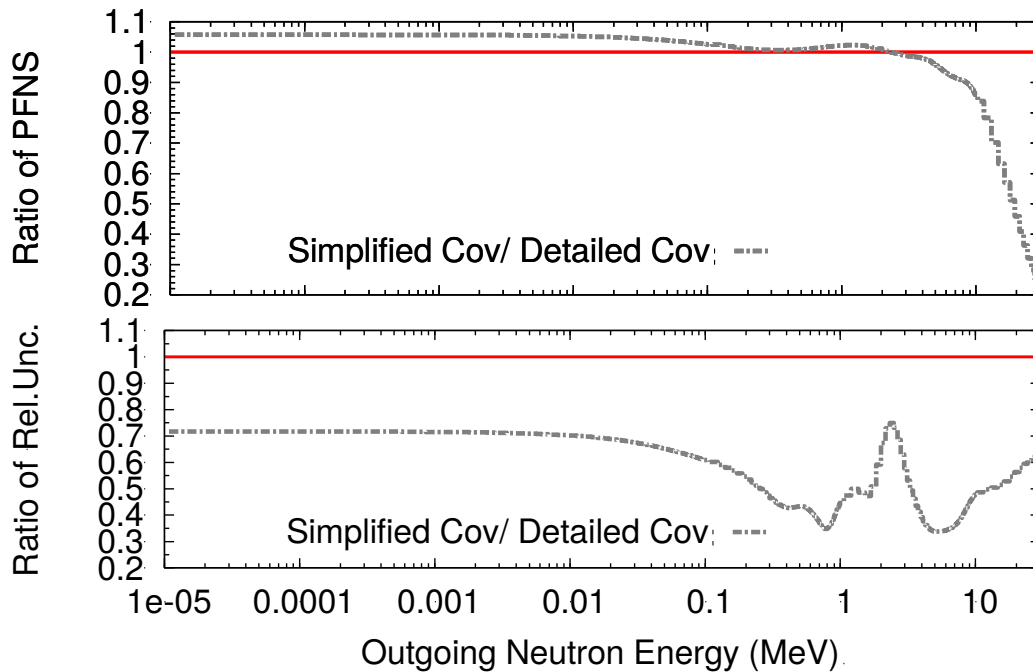
# Simplified vs detailed uncertainty estimate leads to distinct change of evaluated PFNS.



# Simplified versus detailed uncertainty leads to significantly underestimated evaluated unc.



# Simplified versus detailed uncertainty estimate significantly impacts benchmark results.



**Change in Jezebel  $k_{\text{eff}}$ :  
195 pcm !!!**

**Drop in Jezebel  $k_{\text{eff}}$   
unc. due to PFNS  
uncertainty:  
-69% !!!**