LA-UR-24-32087

Approved for public release; distribution is unlimited.

Title: Uncertainty quantification to prepare experimental database for nuclear data evaluations

Author(s): Neudecker, Denise

Intended for: FIESTA2024, 2024-11-18/2024-11-22 (Los Alamos, New Mexico, UNITED STATES)
Web

Issued: 2024-11-12

Uncertainty quantification to prepare experimental database for nuclear data evaluations

D. Neudecker

FIESTA, Nov. 18, 2024

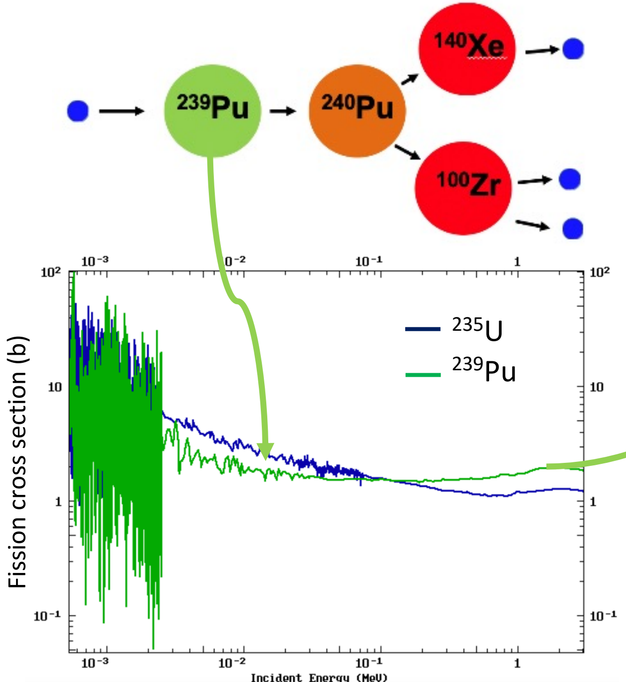
What are we going to learn in this practical session?

- What is nuclear data evaluation?
- Why do we need to prepare an experimental database for the evaluation?
- How do we render experimental data consistent for an evaluation?
- What are we going to do in this tutorial?

What is nuclear data evaluation?

Nuclear data tabulate physics reaction mechanism for use in transport simulations to support nuclear applications.

Nuclear data tabulate physics reaction mechanism of the nucleus.
Example: neutron-induced fission on ^{239}Pu



Nuclear data are required inputs for predictive simulations using e.g., MCNP; they often dominate the total uncertainty of these simulations.

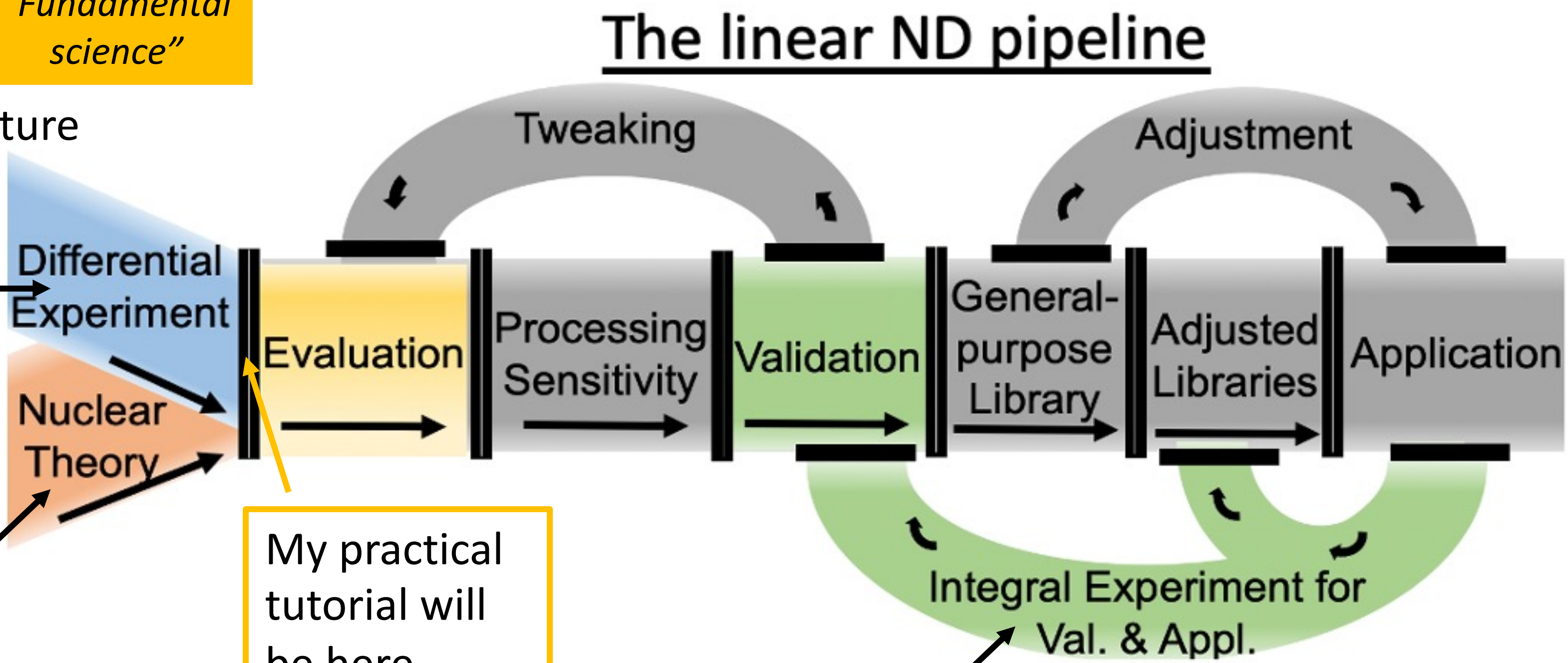
- Nuclear reactor physics
- Nuclear critical and subcritical experiments
- Criticality safety
- Nuclear diagnostics
- Survivability
- Intrinsic radiation
- Radiography
- Nuclear weapon effects and output
- Emergency response / nuclear threat assessments
- Nuclear safeguards and nonproliferation
- Radiation detection and analysis
- Medical and health physics

Nuclear data are produced by a complex pipeline that connects “fundamental” to ”applied” science.

“Fundamental science”

Fredrik’s lecture & Maria’s practical of today

Patrick’s lecture of today



My practical tutorial will be here

Jesson’s & Joetta’s lecture on Friday

“Applied science”

Why do we need to prepare an experimental database for the evaluation?

EXFOR (https://www-nds.iaea.org/exfor/exfor.htm) gives easy access to experimental data for nuclear data evaluations.

https://www-nds.iaea.org/exfor/exfor.htm

Help » Manual | Lexfor | Output | Plot+ | R33   Databases » ENDF | CINDA | IBANDL | EEView   Download » X4Lite | X4Pro | X5json | Catalog | Web-API

NNDC   NRDC

Experimental Nuclear Reaction Data (EXFOR)

Database Version of 2024-10-30

Software Version of 2024-09-20

The EXFOR library contains an extensive compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle and photon reactions have been covered less extensively.

EXFOR Reference Paper: Nucl. Data Sheets 120 (2014) 272, [arxiv].

EXFOR Web database retrieval system provides: data search, output to various formats (incl.XML), plotting and comparison to ENDF, re-normalization old data to new standards, calculating data for inverse reactions and kinematics, constructing correlation matrices from partial uncertainties, etc.

EXFOR Web Database & Tools Paper: NIM A 888 (2018) 31, [arxiv].

The EXFOR database contains data from 25127 experiments (see statistics and recent database updates). Mirror-sites

Search: Go ?

Examples of requests: 1 2 3 4 5 6 7 ...

Request   Submit   Reset   Help

- Target ?
- Reaction ?
- Quantity ?
- Product ?
- Energy from to eV ?
- Author(s) ?
- Publication year ?
- Last modified ?
- Accession # ?

Extended
Keywords
Expert
Evaluator

Submit   Reset

Submit in new Window

Go to: [upload your data]; EE-View:CS,CS1,DA

Options

- [x] Exclude superseded data
- [ ] No reaction combinations (ratios,..)
- [x] Exclude evaluated/calculated data
- [x] Enhanced search of Products
- [ ] Show evaluators flags //2021
- [ ] Retrieve listing only
- [ ] Disable Prompt-help

Sort by: (•) reaction ( ) publication
View: ( ) basic (•) extended

Ranges (Z,A)
Reaction Sub-Fields
Feedback and User's Input

Clone Request:
CINDA   ENDF

More Web Tools

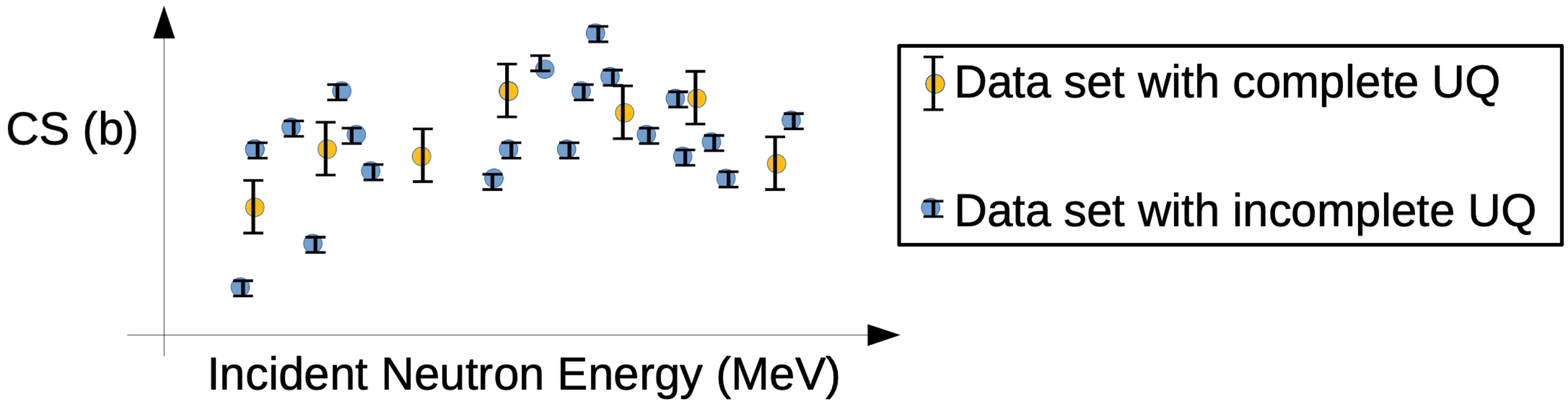
Plotting. See also: [video-guide]

Note:
- all criteria are optional (selected by checking ☑)
- selected criteria are combined for search with logical AND
- criteria separated in a field by ";" are combined with logical OR
- criteria starting with "^" will be used as logical NOT
- wildcards (*) and intervals (..) are available

Database Manager: Naohiko Otsuka, NDS, International Atomic Energy Agency (n.otsuka@iaea.org)
Web and Database Programming: Viktor Zerkin, NDS, International Atomic Energy Agency (nds.contact-point@iaea.org) 2024-09-20
Data Source: International Network of Nuclear Reaction Data Centres (NRDC)

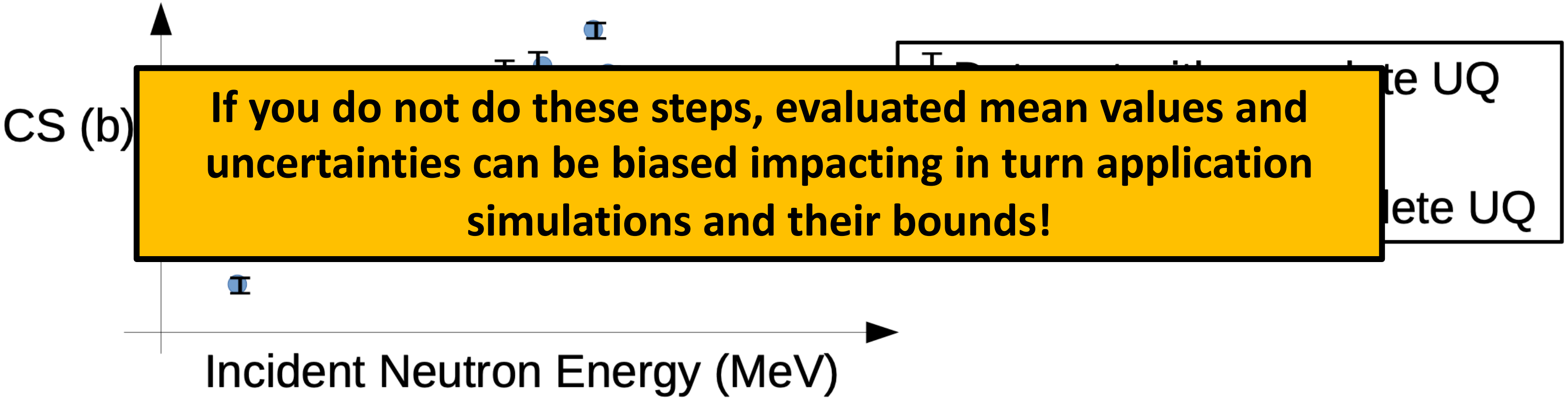
BUT, one cannot adopt data blindly from EXFOR. One needs to:

- Remove clear outliers from experimental database.
- Renormalize data to the newest standard if measured as ratios to those.
- Undertake detailed uncertainty quantification ***for each dataset in the database*** to ensure that they have justified weight with respect to each other.
- Critically assess all data in the database and reject data that cannot be trusted given bias in the data or flags when reading the literature.



BUT, one cannot adopt data blindly from EXFOR. One needs to:

- Remove clear outliers from experimental database.
- Renormalize data to the newest standard if measured as ratios to those.
- Undertake detailed uncertainty quantification ***for each dataset in the database*** to ensure that they have justified weight with respect to each other.
- Critically assess all data in the database and reject data that cannot be trusted given bias in the data or flags when reading the literature.



If you do not do these steps, evaluated mean values and uncertainties can be biased impacting in turn application simulations and their bounds!

How do we render experimental data consistent for an evaluation?

Templates of expected measurement uncertainties can help complete uncertainties for curated database.

Templates:
- Document what experiment information and uncertainty sources are needed for evaluators to make most use of experimental data stored in EXFOR.
- Provide stand-in values for uncertainty sources that are not provided by experimenters.

Template's benefit:
- Evaluators can make **more informed choices to fill in missing uncertainty** and correlation information.
- Leads to a **more balanced uncertainty quantification across different data sets.**

Applying templates for UQ leads to more realistic evaluated uncertainties for nuclear data libraries.

Where are templates documented?

General introduction	D. Neudecker et al., EPJ N 9, 35 (2023) , https://doi.org/10.1051/epjn/2023014
Fission cross section	D. Neudecker et al., NDS 163, 228 (2020), https://doi.org/10.1016/j.nds.2019.12.005
Total cross section	A. Lewis et al., EPJ N 9, 34 (2023) , **https://doi.org/10.1051/epjn/2023018**
Capture and charged particle cross section	A. Lewis et al., EPJ N 9, 33 (2023) , **https://doi.org/10.1051/epjn/2023015**
Scattering cross section	J. Vanhoy et al., EPJ N 9, 31 (2023) , **https://doi.org/10.1051/epjn/2023019**
Neutron multiplicity	D. Neudeckeret al., EPJ N 9, 30 (2023) , **https://doi.org/10.1051/epjn/2023016**
Prompt fission neutron spectrum	D. Neudecker et al., EPJ N 9, 32 (2023) , **https://doi.org/10.1051/epjn/2023013**
Fission yields	E. Matthews, *Advancements in the nuclear data of fission yields*, PhD thesis, Department of Nucl. Engineering, University of California, Berkeley, USA, 2021.

We will work today with the (n,f) cross section template.

General introduction	**D. Neudecker et al., EPJ N 9, 35 (2023) , https://doi.org/10.1051/epjn/2023014**
Fission cross section	D. Neudecker et al., NDS 163, 228 (2020), https://doi.org/10.1016/j.nds.2019.12.005
Total cross section	A. Lewis et al., EPJ N 9, 34 (2023) , **https://doi.org/10.1051/epjn/2023018**
Capture and charged particle cross section	A. Lewis et al., EPJ N 9, 33 (2023) , **https://doi.org/10.1051/epjn/2023015**
Scattering cross section	J. Vanhoy et al., EPJ N 9, 31 (2023) , **https://doi.org/10.1051/epjn/2023019**
Neutron multiplicity	D. Neudeckeret al., EPJ N 9, 30 (2023) , **https://doi.org/10.1051/epjn/2023016**
Prompt fission neutron spectrum	D. Neudecker et al., EPJ N 9, 32 (2023) , **https://doi.org/10.1051/epjn/2023013**
Fission yields	E. Matthews, *Advancements in the nuclear data of fission yields*, PhD thesis, Department of Nucl. Engineering, University of California, Berkeley, USA, 2021.

And here is the template:

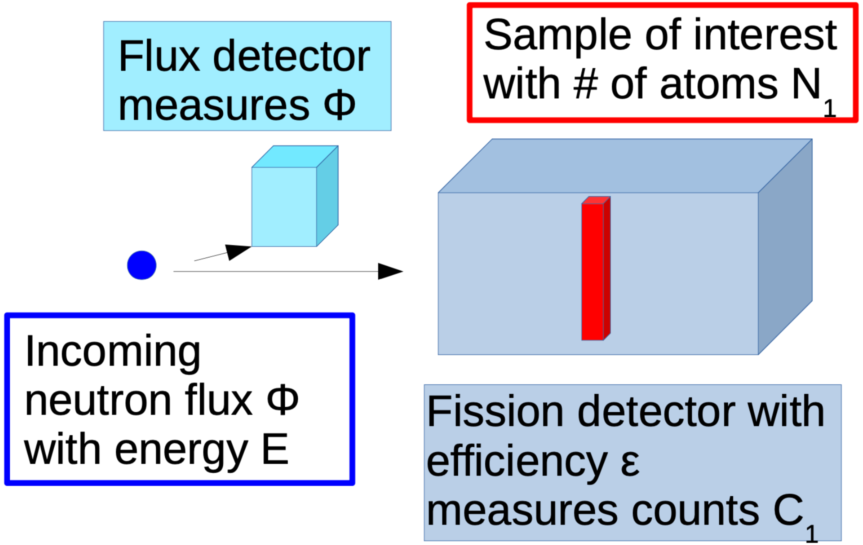
Table 2: Typical uncertainty sources encountered in (n,f) measurements that involve detecting fission fragments are listed dependent on their specific measurement type. The amendments from the preliminary version of the template in Ref. [9] are highlighted in red.

Normalization
Counting Statistics
Multiple scattering
Efficiency
Background
Energy
Flux
Impurity
Deadtime

Unc. source	Absolute	Absolute clean ratio	Absolute indirect ratio
$\delta N_{(a/b\&c)}$	See Table 1	Both samples	Both samples
δc	Eqs. (3) and (5)	Both, combined	Both, combined
$\delta\beta$ & δm; δm	0.2–2%	0.02–0.2%	0.2–2%
$\delta\beta$ & δm; $\delta\beta$	0.2–1%	Less than absolute	0.2–1%
$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1–4%	0.3–4%	1.1-4%, 0.5–1%
$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Compare to nuclear data	Compare to nuclear data
δb	0.2–>10%	0.2–>10%	0.2–>10%
δE	1%, 1-3 ns	Combined	Both detectors
$\delta\phi$	>1%	Cancels or small	Cancels or small
$\delta\zeta$	See Table 3	See Table 3	See Table 3
δd	>0.1%	Both combined	Both detectors

The tutorial covers this measurement type.

Absolute cross section experiments determine the (n,f) cross section directly.



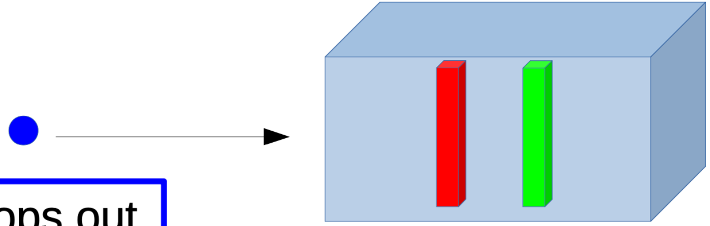
$$\sigma(E) = \frac{C_1(E)}{\Phi(E)\,\epsilon(E)\,N_1}\,\zeta(E)$$

We'll talk about the corrections ζ later.

In clean ratio measurement, the (n,f) cs are measured relative to a reference cross section with the same detector.

Sample of interest with # of atoms N_1

Reference sample with # of atoms N_2



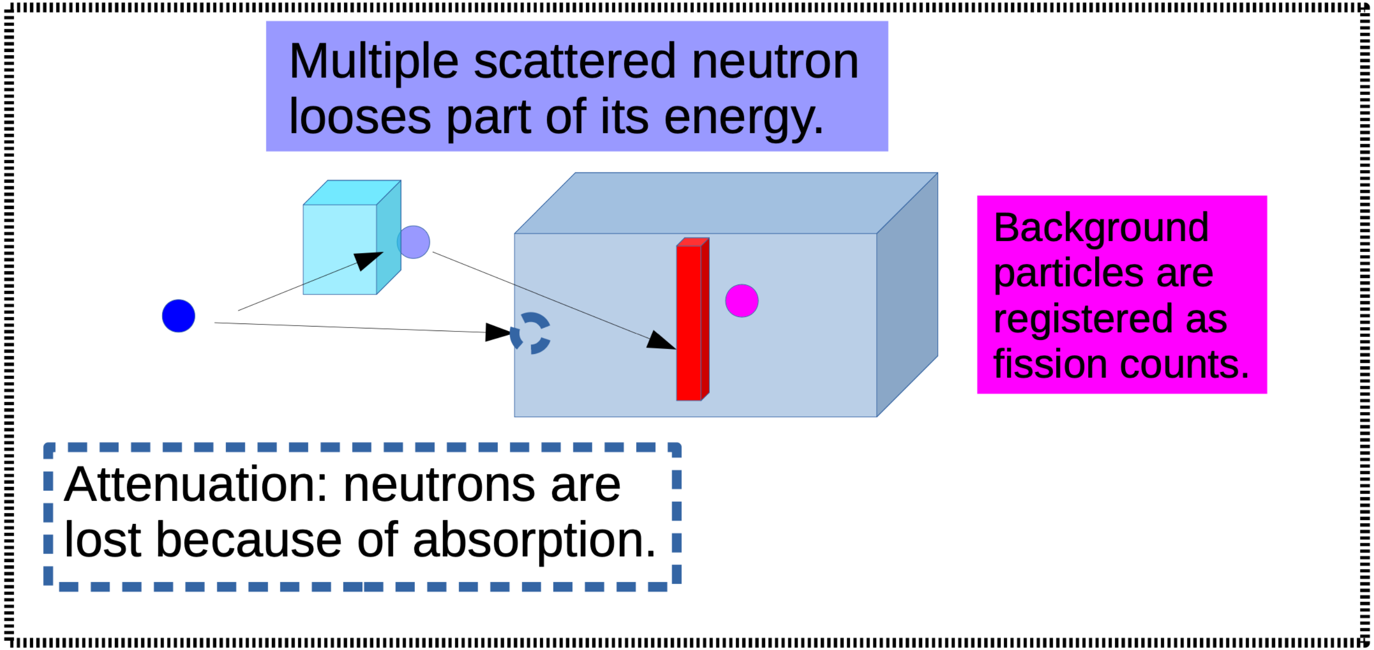
Φ drops out

ε reduces to a correction factor $\delta\varepsilon$ for the two samples.

$$\sigma(E)=\sigma_R^{ND}(E)\frac{C_1(E)N_2}{C_2(E)N_1}\delta\epsilon(E)\zeta(E)$$

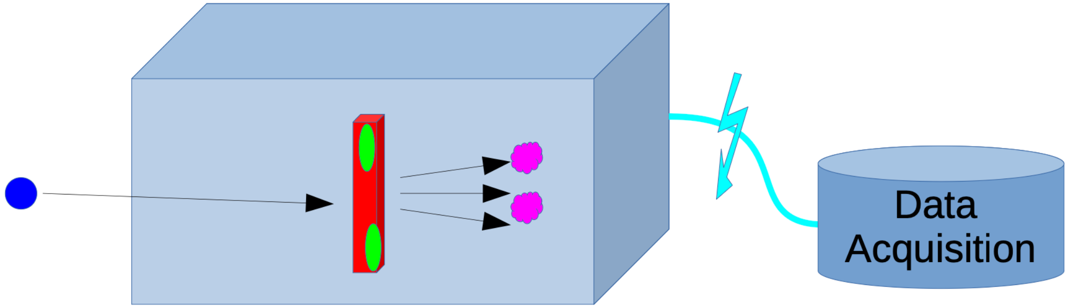
The nuclear data of the reference data σ_R^{ND} is needed to get σ.

Corrections due to measurement environment: background, multiple scattering and attenuation.



$$\sigma(E)=\frac{C_1(E)-C_b}{\Phi(E)\epsilon(E)N_1}\delta\beta(E)\delta m(E)\zeta'(E)$$

Other corrections: deadtime and impurity.



Deatime τ: detector cannot record any counts within a short time window after detecting counts.

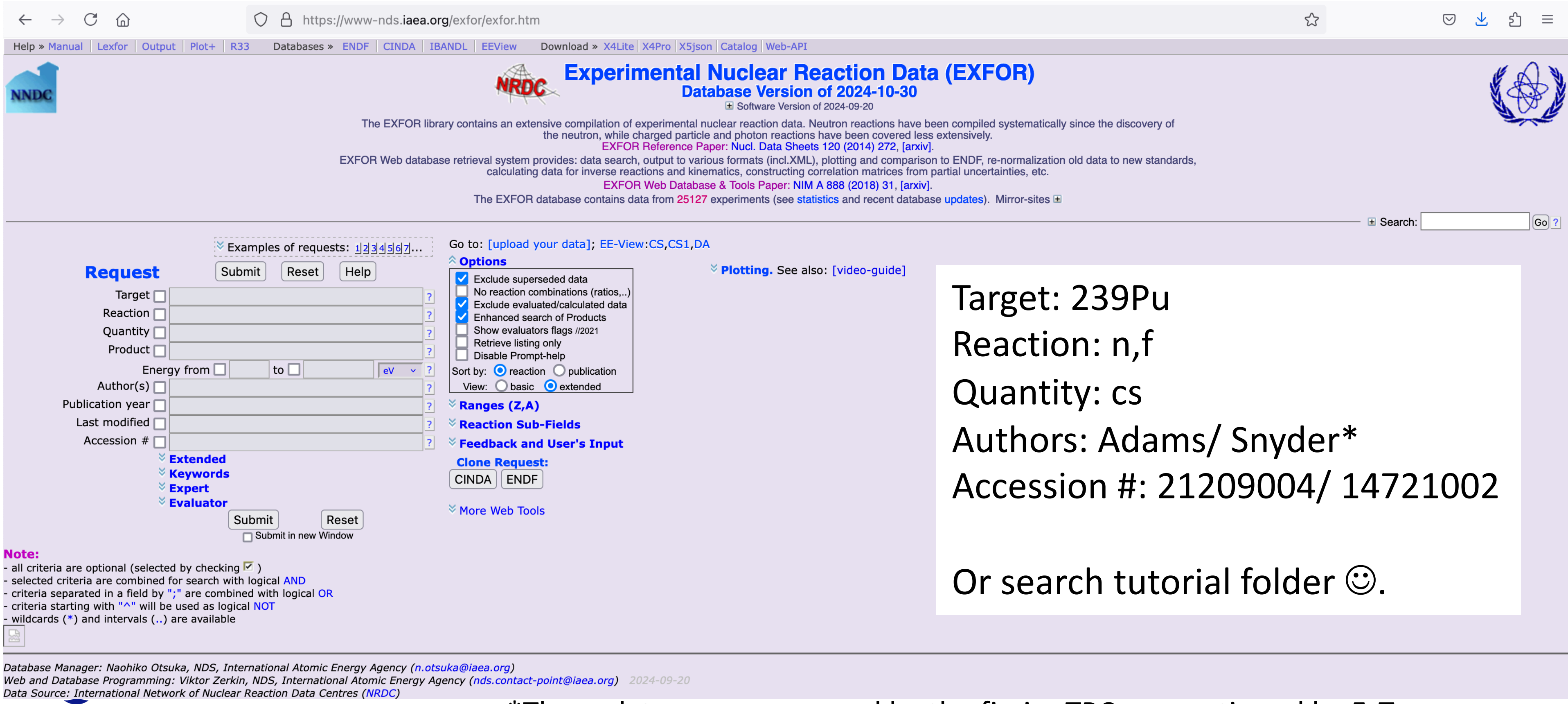
Impurities in the sample: counts are detected from fission σ_{ip} from impurities in the sample with number of atoms N_{ip}

$$\sigma(E)=\frac{C_1(E)}{\Phi(E)\epsilon(E)N_1\tau}\zeta''(E)\left[1+\sum_p \sigma_{ip}(E)N_{ip}\right]^{-1}$$

What are we going to do in this tutorial? – Retrace the steps to prepare a database for nuclear data evaluation.

1. Find two data sets in EXFOR.
2. Re-normalize data with newest standard.
3. Plot the renormalized data with uncertainties straight from EXFOR.
4. Apply the templates to see if all uncertainties are provided.
5. Estimate total covariances using templates.
6. Re-plot the data.
7. Bonus point: Figure out what uncertainties are still missing.

1. Go to EXFOR: https://www-nds.iaea.org/exfor/exfor.htm and find ^{239}Pu(n,f) cs data by Adams et al. & Snyder et al.

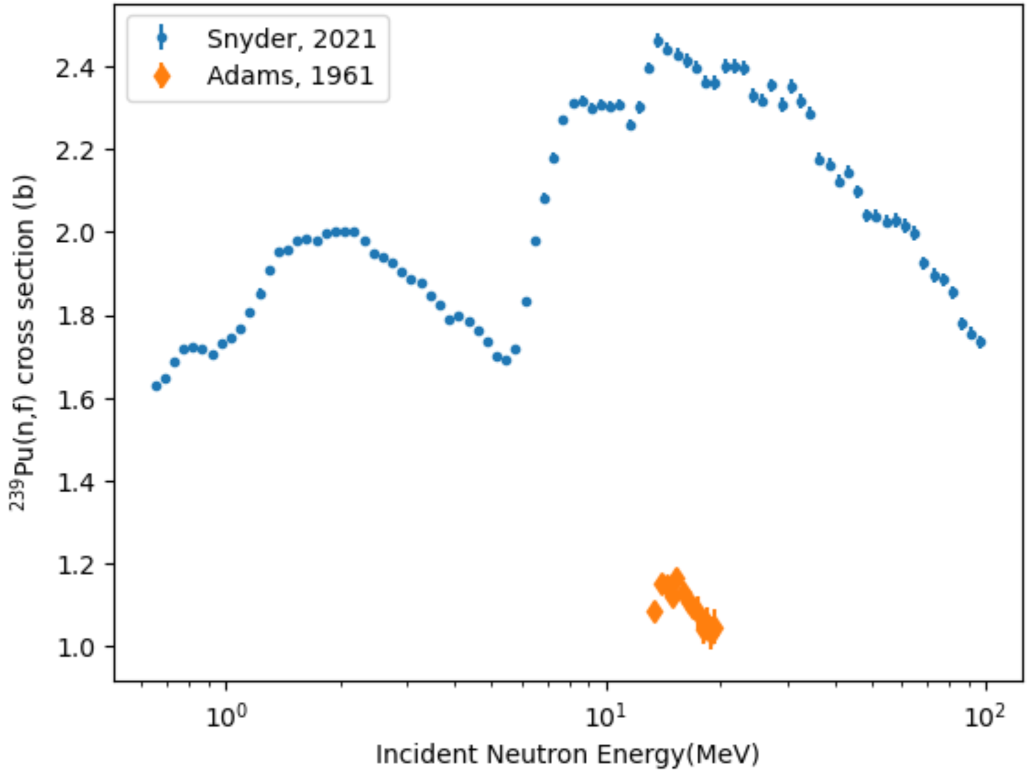


Target: 239Pu
Reaction: n,f
Quantity: cs
Authors: Adams/ Snyder*
Accession #: 21209004/ 14721002

Or search tutorial folder ☺.

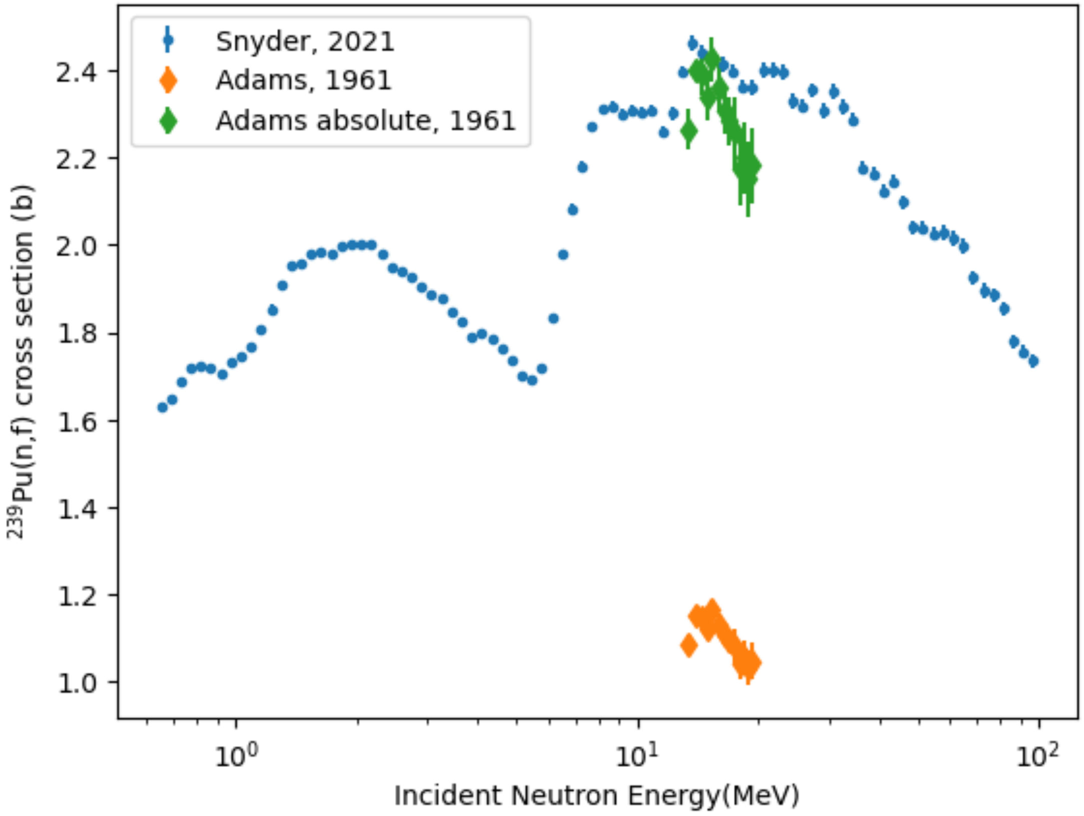
*These data were measured by the fissionTPC as mentioned by F. Tovesson.

2. Renormalize the data with the newest standard. 3. Plot the renormalized data with uncertainties from EXFOR.



- There are clearly some discrepancies in the data!
- **To-do: Read the EXFOR entries and figure out why we see such large discrepancies (3 minutes).**

Solution: Adams data are shape data. Ratio data are set to 1.0 at 14.0 MeV. Re-normalize to current evaluation.



- Renormalizing ratio data with factor 2.4/1.151 as this aligns the cross section with the VIII.1 ^{239}Pu(n,f) cs.
- We still see distinct discrepancies.
- Maybe, some uncertainties are missing?

In shape measurement, the normalization N is not defined. The shape cross section floats with respect to y-axis.

Shape measurement: $$\Sigma(E) = \frac{C_1(E)}{\Phi(E)\epsilon(E)}\zeta(E)$$

Clean ratio shape measurement: $$\Sigma(E) = \sigma_R^{ND}(E)\frac{C_1(E)}{C_2(E)}\delta\epsilon(E)\zeta(E)$$

Indirect ratio shape measurement: $$\Sigma(E) = \sigma_R^{ND}(E)\frac{C_1(E)\epsilon_2(E)}{C_2(E)\epsilon_1(E)}\delta\zeta(E)$$

4. To-do: Counter-check with the templates if all unc. are provided in EXFOR and fill in missing ones via templates.

Table 2: Typical uncertainty sources encountered in (n,f) measurements that involve detecting fission fragments are listed dependent on their specific measurement type. The amendments from the preliminary version of the template in Ref. [9] are highlighted in red.

	Unc. source	Absolute	Absolute clean ratio	Absolute indirect ratio
Normalization	$\delta N_{(a/b\&c)}$	See Table 1	Both samples	Both samples
Counting Statistics	δc	Eqs. (3) and (5)	Both, combined	Both, combined
Multiple scattering	$\delta\beta$ & δm; δm	0.2–2%	0.02–0.2%	0.2–2%
	$\delta\beta$ & δm; $\delta\beta$	0.2–1%	Less than absolute	0.2–1%
Efficiency	$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1–4%	0.3–4%	1.1–4%, 0.5–1%
	$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Compare to nuclear data	Compare to nuclear data
Background	δb	0.2–>10%	0.2–>10%	0.2–>10%
Energy	δE	1%, 1-3 ns	Combined	Both detectors
Flux	$\delta\phi$	>1%	Cancels or small	Cancels or small
Impurity	$\delta\zeta$	See Table 3	See Table 3	See Table 3
Deadtime	δd	>0.1%	Both combined	Both detectors

Lessons learned: (a) it is more the rule than exception that unc. are missing, (b) synonyms complicate applying templates

<u>Solution Snyder: Many unc. provided</u>

```
statuncSny         = alldata[:,5]
multscattuncSny    = alldata[:,11]
efficiencyuncSny1 = alldata[:,8]
efficiencyuncSny2 = alldata[:,6]
backgrounduncSny  = alldata[:,7]
fluxuncSny         = alldata[:,10]
impurityuncSny     = alldata[:,9]
deadtimeuncSny     = 0.0*Esny # article
normuncSny         = ones(shape(ESny)[0],dtype=float)*1.41
# templates;  https://doi.org/10.1016/j.nima.2021.165864) not recorded in EXFOR
gives 0.288%.
```

Lessons learned: (a) it is more the rule than exception that unc. are missing, (b) synonyms complicate applying templates

<u>Solution Adams: Many unc. missing</u>

```
alldata = loadtxt('Adams_EXFORNo21209004.txt'); dim = shape(alldata)[0]
statuncAd        = alldata[:,2]*100.0/alldata[:,1]
multscattuncAd   = ones(dim,dtype=float)*0.5 # from templates
efficiencyuncAd  = ones(dim,dtype=float)*4.0 # from templates (I assume the high number because the samples were not in the same detector)
backgrounduncAd  = ones(dim,dtype=float)*5.0 # from templates (I assume a high number because a high alpha background was mentioend).
fluxuncAd        = ones(dim,dtype=float)*0.0 # from template, also flux was monitored with two detectors.
impurityuncAd    = ones(dim,dtype=float)*sqrt(0.3*0.3+0.6*0.6) # from template, look at sample contaminants and then table 3.
deadtimeuncAd    = 0.0*ESny     # from journal article
normuncAd        = zeros(dim,dtype=float) # because a shape measurement
```

5. Estimate total covariances using templates.

A covariance matrix is 2^{nd} moment of probability distribution.

A probability density function $p(x_1,x_2)$ gives the "complete information" for these two variables.

<u>First Moment:</u> Mean value

$$\langle x_1\rangle=\iint x_1\,p(x_1,x_2)\,dx_1\,dx_2 \qquad \langle x_2\rangle=\iint x_2\,p(x_1,x_2)\,dx_1\,dx_2$$

<u>Second Moment:</u> Variances and covariances

$$var(x_1)=\iint (x_1-\langle x_1\rangle)^2\,p(x_1,x_2)\,dx_1\,dx_2$$

$$var(x_2)=\iint (x_2-\langle x_2\rangle)^2\,p(x_1,x_2)\,dx_1\,dx_2$$

$$\boxed{cov(x_1,x_2)=\iint (x_1-\langle x_1\rangle)(x_2-\langle x_2\rangle)\,p(x_1,x_2)\,dx_1\,dx_2}$$

The correlation matrix normalizes the linear dependence of x_1 and x_2 to be between 1 and -1.

$$\boxed{cor(x_1, x_2) = \frac{cov(x_1, x_2)}{\sqrt{var(x_1)\, var(x_2)}}}$$

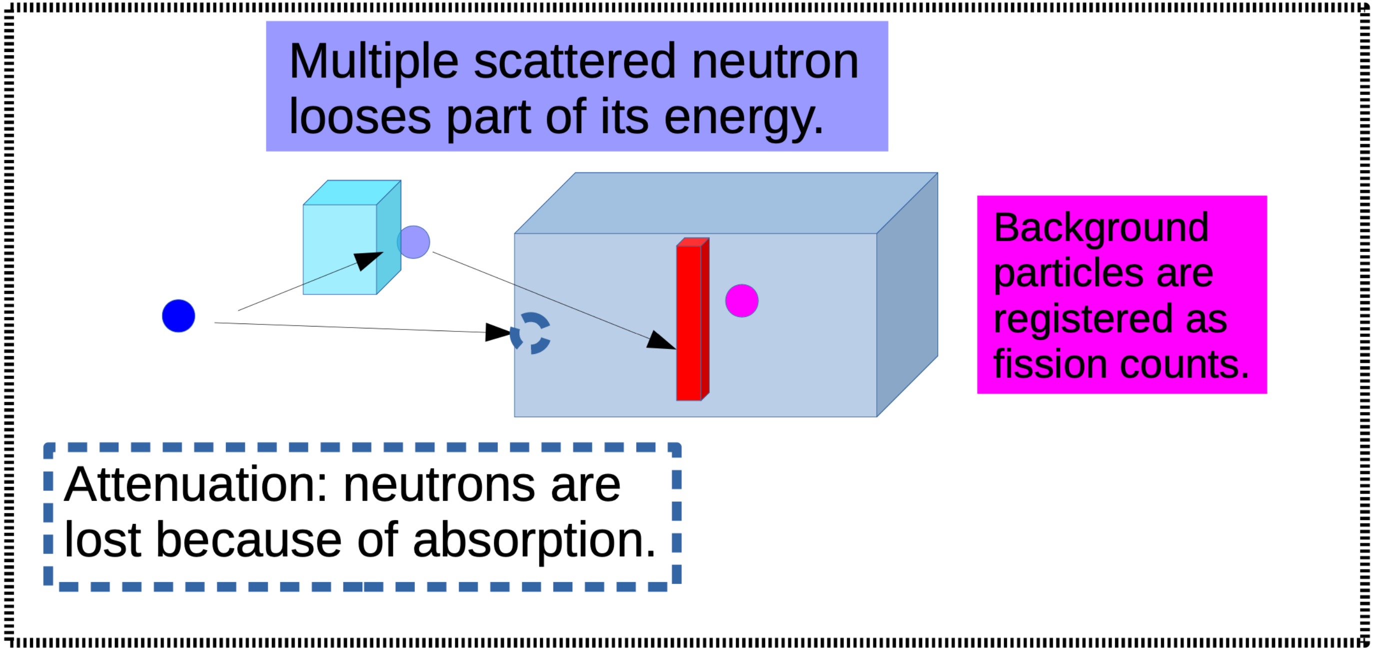
Properties:

- ❑ $-1 \leq cor(x_1, x_2) \leq 1$
- ❑ Diagonal always 1
- ❑ Positive semi-definite
- ❑ Symmetric

Correlations:

- ❑ 0: uncorrelated behavior.
- ❑ 1: full correlation.
- ❑ -1: anti-correlation.

We combine $var^k(x_1)$ and $cor^k(x_1,x_2)$ for k distinct uncertainty sources to total covariances $Cov(x_1,x_2)$



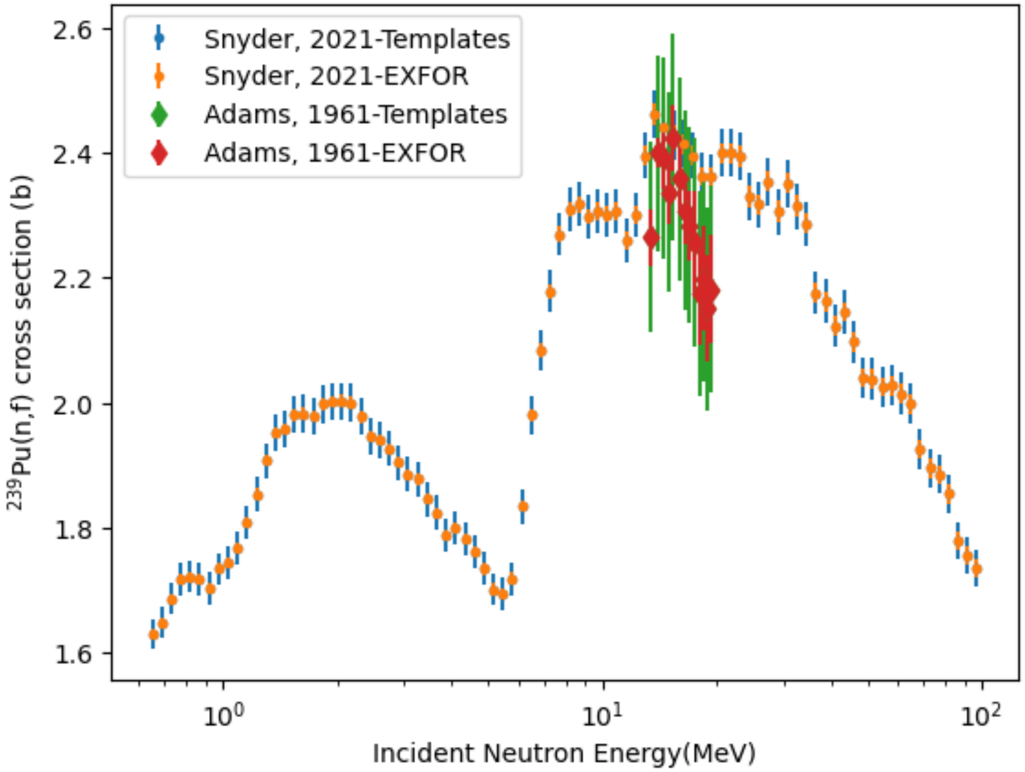
$$Cov^{exp} = Cov^{Count.\ Stat.} + \boxed{Cov^{Backgd.}} + Cov^{Mult.\ Scatt.} + \boxed{Cov^{TOF}} + \boxed{Cov^{Det.\ Eff.}} + \ldots$$

Correlation functions are proposed in the templates paper as they are rarely provided in the literature.

Unc. source	Typical range	Cor(Exp$_i$,Exp$_i$)	Cor(Exp$_i$, Exp$_j$) $i \neq j$
$\delta N_{(a)}$	$> 1\%$	Full	$\neq 0$ if same technique/sample
$\delta N_{(b\&c)}$	0-0.5% (Vapor-deposited target)	Full	$\neq 0$ if same technique/sample
	1% (Painted/electro-plated target)	Full	$\neq 0$ if same technique/sample
δc	Eqs. (3) and (5)	Diagonal	0
$\delta\beta$ & δm; δm	0.02–2%	Gaussian [20]	0.5–0.75
$\delta\beta$ & δm; $\delta\beta$	0.2–1%	Gaussian	0.5–0.75
$\delta\varepsilon$ & $\delta\alpha$; $\delta\varepsilon$	1.1-4%	Close to full	0.5–1
$\delta\varepsilon$ & $\delta\alpha$; $\delta\alpha$	Compare to nuclear data	Gaussian	0.75–1.0
δb	0.2–>10%	Gaussian	Possible
δE	1%, 1–3 ns (TOF, for given TOF length)	From conversion	Technique-dependent
$\delta\phi$	0%, >1%	0.5–Full	Technique-dependent
$\delta\zeta$	See Table 3	0.9–1	0.5–0.75
δd	>0.1%	Full	0

To-do: estimate total covariances for both data sets.

6. Re-plot the data: the added template uncertainties resulting in data with overlapping uncertainties …



A word of caution: While the uncertainties now overlap, I would still think twice before accepting Adams' data.

7. Bonus point: Figure out what uncertainties are still missing.

When you read through the template list, you realize that two uncertainty sources are missing:

- Those from the standard: We would need to load the covariances from the standards.
- Energy uncertainties: Requires transformation from energy to cross section space.

It is a bit trickier to implement, so try it at home. ☺

Lessons learned:

- Carefully read the EXFOR entry to understand what data is given (absolute and unc.) and what uncertainties are provided.
- Not all relevant information is in EXFOR. If you care about high-quality uncertainty estimate, you need to read each paper and dig deeper.
- Templates can help you fill in missing uncertainties.
- Templates and the journal articles can give you hints at what could drive biases between experiments, but ultimately, evaluators need to decide what data to accept.
- Often, one or more experimental uncertainty sources are missing in EXFOR and/ or the literature.

Establishing an experimental database for evaluations is a distinct step to go from reported experiments to using them in evaluations. Choices made there can influence your evaluated data.

Solution notebook

Uncertainty quantification to prepare experimental database for nuclear data evaluations

[102]:
```
# loading necessary packages
from numpy import array, shape, diag, arange, ones, zeros, loadtxt, sqrt, meshgrid, interp, exp
import matplotlib.pyplot as plt
%matplotlib inline
```

1. Go to EXFOR: https://www-nds.iaea.org/exfor/exfor.htm and find ^{239}Pu(n,f) cs data by Adams et al. & Snyder et al. (or look into tutorial folder).

[33]:
```
# Load data.
ESny = loadtxt('Snyder_EXFORNo14721002.txt')[:,0]*0.5+loadtxt('Snyder_EXFORNo14721002.txt')[:,1]*0.5 # loading energy grid
DataSny = loadtxt('Snyder_EXFORNo14721002.txt')[:,3] # loading ratio data
TotUncSny = loadtxt('Snyder_EXFORNo14721002.txt')[:,4] # loading 1-sigma standard deviations

EAd = loadtxt('Adams_EXFORNo21209004.txt')[:,0] # loading energy grid
DataAd = loadtxt('Adams_EXFORNo21209004.txt')[:,1] # loading ratio data
TotUncAd = loadtxt('Adams_EXFORNo21209004.txt')[:,2] # loading 1-sigma standard deviations
```

2. Renormalize the data with the newest standard:

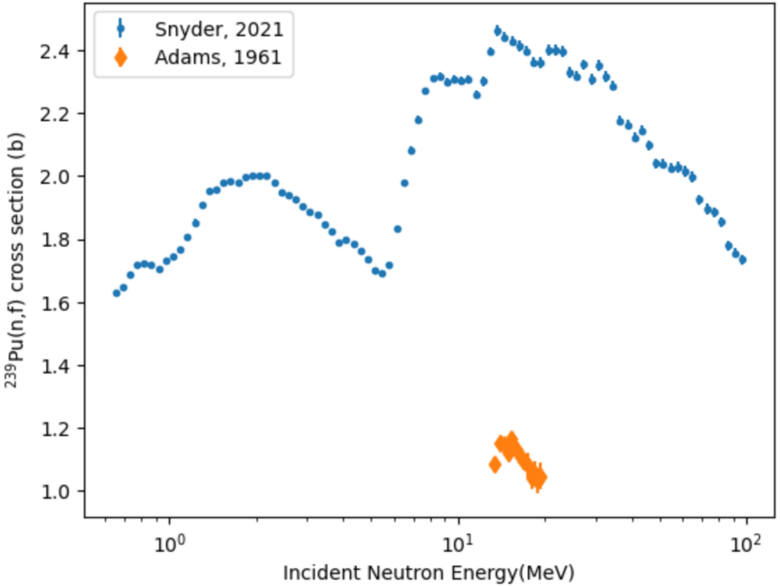
- Load ^{235}U and ^{238}U(n,f) standard cs.
- Renormalize.

[47]:
```
# Load standards.
EU5nfcsstd = loadtxt('Standard_U235nfcs_2017.txt')[:,0]; DataU5nfcsstd = loadtxt('Standard_U235nfcs_2017.txt')[:,1] # U235(n,f) cs
EU8nfcsstd = loadtxt('Standard_U238nfcs_2017.txt')[:,0]; DataU8nfcsstd = loadtxt('Standard_U238nfcs_2017.txt')[:,1] # U238(n,f) cs

# Renormalize with newest standard.
nfcsSny = DataSny*interp(ESny,EU5nfcsstd,DataU5nfcsstd); TotUncnfcsSny = TotUncSny*interp(ESny,EU5nfcsstd,DataU5nfcsstd)
nfcsAd  = DataAd*interp(EAd,EU8nfcsstd,DataU8nfcsstd);   TotUncnfcsAd  = TotUncAd*interp(EAd,EU8nfcsstd,DataU8nfcsstd)
```

3. Plot the renormalized data with uncertainties straight from EXFOR.

[79]:
```
plt.xscale("log")
plt.errorbar(ESny,nfcsSny,yerr=TotUncnfcsSny,fmt='.')
plt.errorbar(EAd,nfcsAd,yerr=TotUncnfcsAd,fmt='d')
#plt.errorbar(EAd,nfcsAd*2.4/1.151,yerr=TotUncnfcsAd*2.4/1.151,fmt='d')
plt.legend(['Snyder, 2021','Adams, 1961'])#,'Adams absolute, 1961'])
plt.xlabel('Incident Neutron Energy(MeV)'); plt.ylabel(r'$^{239}$Pu(n,f) cross section (b)')
```

[79]:
```
Text(0, 0.5, '$^{239}$Pu(n,f) cross section (b)')
```



4. Counter-check with the templates if all uncertainties are provided:

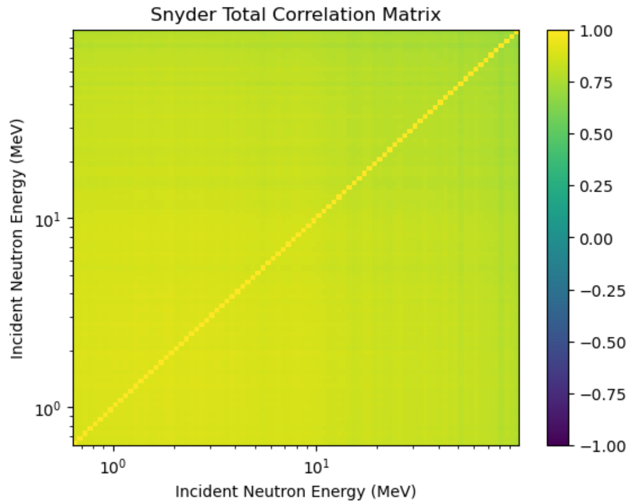
- First Snyder data.
- Then, Adam's data

[98]:
```
alldata = loadtxt('Snyder_EXFORNo14721002.txt')
# all uncertainties are given in %
statuncSny         = alldata[:,5]
multscattuncSny    = alldata[:,11]
efficiencyuncSny1  = alldata[:,8]
efficiencyuncSny2  = alldata[:,6]
backgrounduncSny   = alldata[:,7]
fluxuncSny         = alldata[:,10]
impurityuncSny     = alldata[:,9]
deadtimeuncSny     = 0.0*ESny     # from journal article
normuncSny         = ones(shape(ESny)[0],dtype=float)*1.41 # from templates,
# accompanying journal arictle (https://doi.org/10.1016/j.nima.2021.165864) not recorded in EXFOR gives 0.288%.
```

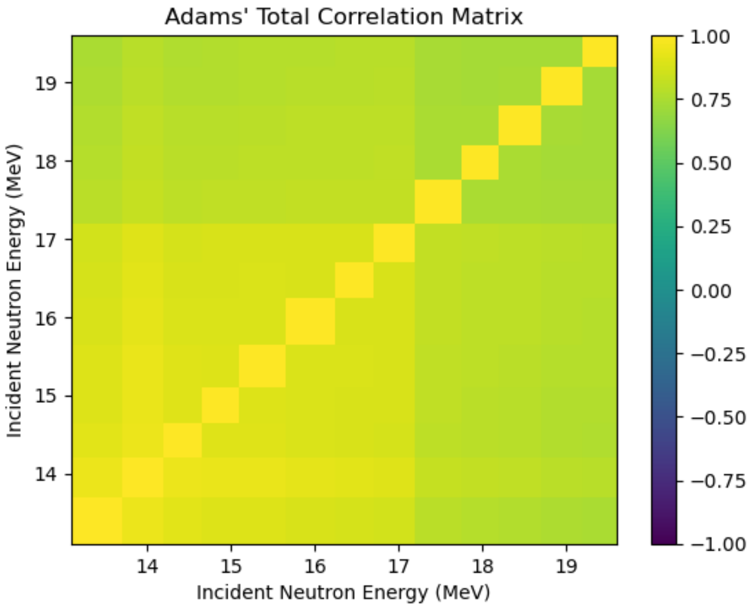
[93]:
```
alldata = loadtxt('Adams_EXFORNo21209004.txt'); dim = shape(alldata)[0]
statuncAd        = alldata[:,2]*100.0/alldata[:,1]
multscattuncAd   = ones(dim,dtype=float)*0.5 # from templates
efficiencyuncAd  = ones(dim,dtype=float)*4.0 # from templates (I assume the high number because the samples were not in the same detector)
backgrounduncAd  = ones(dim,dtype=float)*5.0 # from templates (I assume a high number because a high alpha background was mentioend).
fluxuncAd        = ones(dim,dtype=float)*0.0 # from template, also flux was monitored with two detectors.
impurityuncAd    = ones(dim,dtype=float)*sqrt(0.3*0.3+0.6*0.6) # from template, look at sample contaminants and then table 3.
deadtimeuncAd    = 0.0*ESny     # from journal article
normuncAd        = zeros(dim,dtype=float) # because a shape measurement
```

5. Estimate total covariances using templates.

```
CovSny = zeros([shape(ESny)[0],shape(ESny)[0]],dtype=float)
CorSny = zeros([shape(ESny)[0],shape(ESny)[0]],dtype=float)

for index1 in arange(0,shape(ESny)[0]):
    for index2 in arange(0,shape(ESny)[0]):
        dscr = ((ESny[index1]-ESny[index2])/(max(ESny[index1],ESny[index2])))**2.0

        CovSny[index1,index2] = normuncSny[index1]*normuncSny[index2] + \
        deadtimeuncSny[index1]*deadtimeuncSny[index2] + \
        impurityuncSny[index1]*impurityuncSny[index2] + \
        multscattuncSny[index1]*multscattuncSny[index2]*exp(-1.0*dscr) +\
        backgrounduncSny[index1]*backgrounduncSny[index2]**exp(-1.0*dscr)
    CovSny[index1,index1] = CovSny[index1,index1]+statuncSny[index1]**2.0+fluxuncSny[index1]**2.0+\
    efficiencyuncSny1[index1]**2.0+efficiencyuncSny2[index1]**2.0 # comment, this is from a journal aritcle

TotuncSny = sqrt(diag(CovSny))

for index1 in arange(0,shape(ESny)[0]):
    for index2 in arange(0,shape(ESny)[0]):
        CorSny[index1,index2] = CovSny[index1,index2]/(TotuncSny[index1]*TotuncSny[index2])

x,y = meshgrid(ESny,ESny)
plt.xscale("log")
plt.yscale("log")
plt.xlabel("Incident Neutron Energy (MeV)")
plt.ylabel("Incident Neutron Energy (MeV)")
plt.pcolormesh(x,y,CorSny,vmin=-1, vmax=1)
plt.colorbar()
plt.title("Impurity")
```



```python
CovAd = zeros([shape(EAd)[0],shape(EAd)[0]],dtype=float)
CorAd = zeros([shape(EAd)[0],shape(EAd)[0]],dtype=float)

for index1 in arange(0,shape(EAd)[0]):
    for index2 in arange(0,shape(EAd)[0]):
        dscr = ((EAd[index1]-EAd[index2])/(max(EAd[index1],EAd[index2])))**2.0

        CovAd[index1,index2] = normuncAd[index1]*normuncAd[index2] + \
        deadtimeuncAd[index1]*deadtimeuncAd[index2] + \
        impurityuncAd[index1]*impurityuncAd[index2] + \
        efficiencyuncAd[index1]*efficiencyuncAd[index2] + \
        multscattuncAd[index1]*multscattuncAd[index2]*exp(-1.0*dscr) +\
        backgrounduncAd[index1]*backgrounduncAd[index2]**exp(-1.0*dscr)
    CovAd[index1,index1] = CovAd[index1,index1]+statuncAd[index1]**2.0+fluxuncAd[index1]**2.0

TotuncAd = sqrt(diag(CovAd))

for index1 in arange(0,shape(EAd)[0]):
    for index2 in arange(0,shape(EAd)[0]):
        CorAd[index1,index2] = CovAd[index1,index2]/(TotuncAd[index1]*TotuncAd[index2])

x,y = meshgrid(EAd,EAd)
plt.xlabel("Incident Neutron Energy (MeV)")
plt.ylabel("Incident Neutron Energy (MeV)")
plt.pcolormesh(x,y,CorAd,vmin=-1, vmax=1)
plt.colorbar()
plt.title("Adams' Total Correlation Matrix")
```



6. Plot the renormalized data with uncertainties straight from EXFOR versus new uncertainties.

```
plt.xscale("log")
plt.errorbar(ESny,nfcsSny,yerr=TotuncSny*nfcsSny/100.0,fmt='.')
plt.errorbar(ESny,nfcsSny,yerr=TotUncnfcsSny,fmt='.')
plt.errorbar(EAd,nfcsAd,yerr=TotuncAd*nfcsAd/100.0,fmt='d')
plt.errorbar(EAd,nfcsAd,yerr=TotUncnfcsAd,fmt='d')
plt.legend(['Snyder, 2021-Templates','Snyder, 2021-EXFOR','Adams, 1961-Templates','Adams, 1961-EXFOR'])#,'Adams absolute, 1961'])
plt.xlabel('Incident Neutron Energy(MeV)'); plt.ylabel(r'$^{239}$Pu(n,f) cross section (b)')
```

```
Text(0, 0.5, '$^{239}$Pu(n,f) cross section (b)')
```