International Atomic Energy Agency

Direct use of EXFOR Exchange Files for Fast Neutron Fission Cross Section Evaluation

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1 IAEA Nuclear Data Section

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References:

[1] N. Otuka, O. Iwamoto, "EXFOR-based simultaneous evaluation of neutron-induced uranium and plutonium fission cross sections for JENDL-5" (J. Nucl. Sci. Technol. **59**(2022)1004 https://doi.org/10.1080/00223131.2022.2030259)

[2] N. Otuka, O. Iwamoto, "EXFOR-based simultaneous evaluation of neutron-induced uranium and plutonium fission cross sections for JENDL-5: Inputs and outputs" (JAEA-Data/Code 2022-005=INDC(SEC)-0112 (Rev.), 2022 https://doi.org/10.11484/jaea-data-code-2022-005)

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- Outline of simultaneous evaluation
- Absolute fission cross sections from TUD-KRI collaboration
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Outline of Simultaneous Evaluation

Background and Tasks of This Work

- **Quality of EXFOR entries has a strong impact on evaluation by least-squares analysis.**

- I updated EXFOR entries of ^{233,235,238}U and ^{239,240,241}Pu (n,f) for fast neutrons:

  - Revisions of EXFOR entries by addition of missing information, exclusion of two datasets from same measurement, formatting.

  - Processing of the updated EXFOR entries by reformatting and covariance construction by a script.

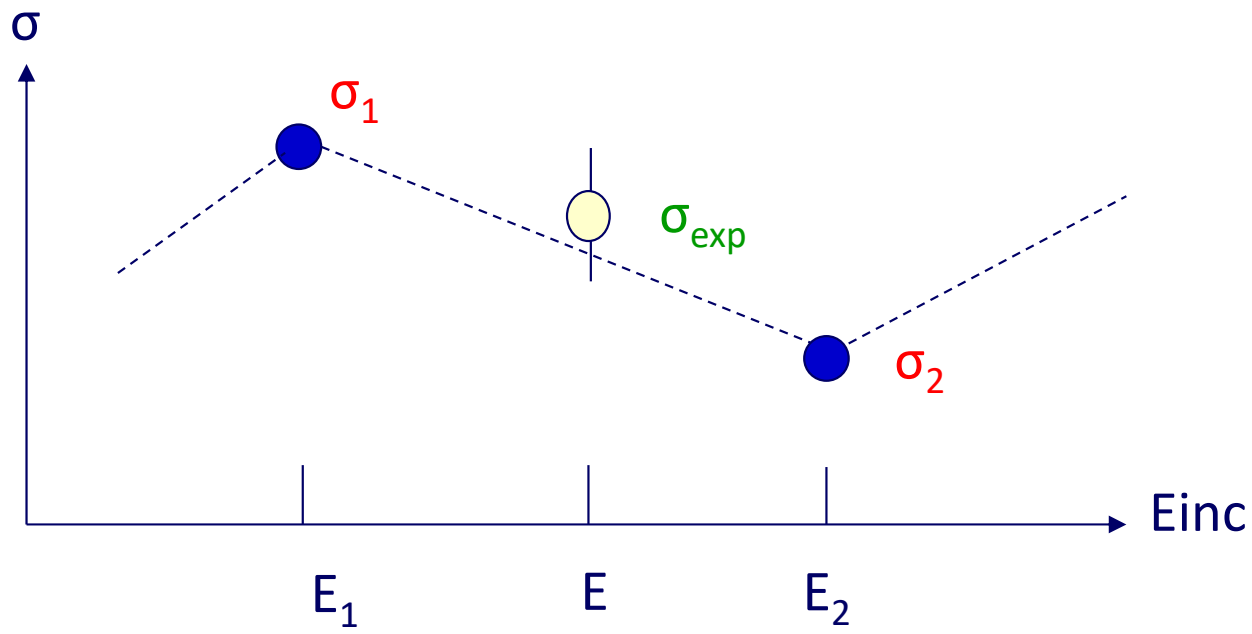
  - Application of the updated EXFOR entries to least-squares analysis (but not for standard/reference purpose)

Selection of Experimental Datasets

- ^{235}U: **1980** to present. Other nuclides: **1970** to present.

- Following datasets were discarded in general:
  - Data read (digitized) from article figures
  - Data compiled without partial uncertainties
  - Data from nuclear explosion

Fitting Procedure

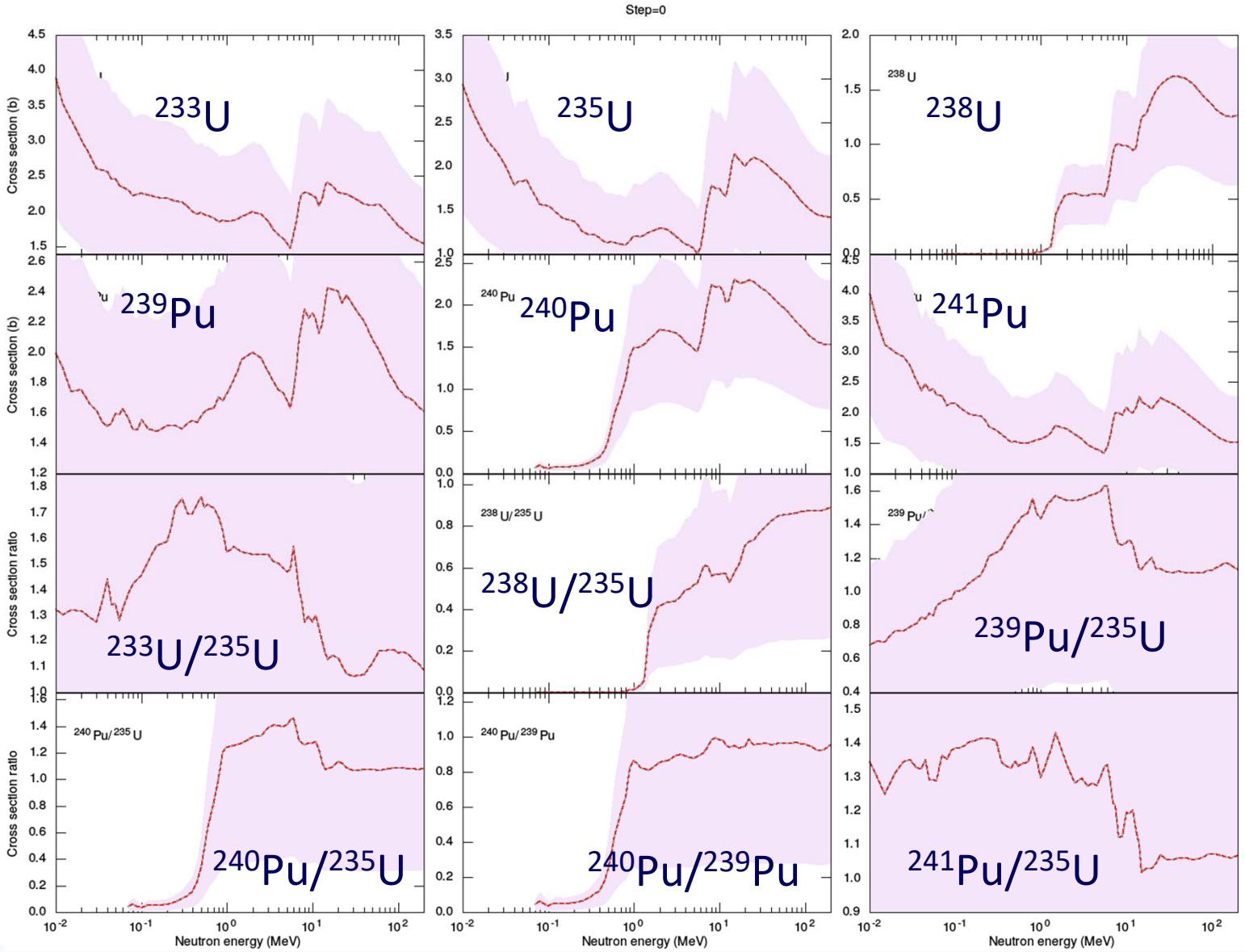


$$\sigma_{exp} \sim [(E-E_1)/(E_2-E_1)]\ \sigma_1 + [(E_2-E)/(E_2-E_1)]\ \sigma_2$$

$$(= 0.5\ \sigma_1 + 0.5\ \sigma_2 \text{ if E is the middle between } E_1 \text{ and } E_2)$$

Evaluated cross sections σ_1 and σ_2 are adjusted to reproduce many σ_{exp} between E_1 and E_2. (Here only one experimental point is shown for simplicity.)

Fitting by Adding EXFOR Datasets
(Update with Exp. Data in Chronological Order 1970→2022)



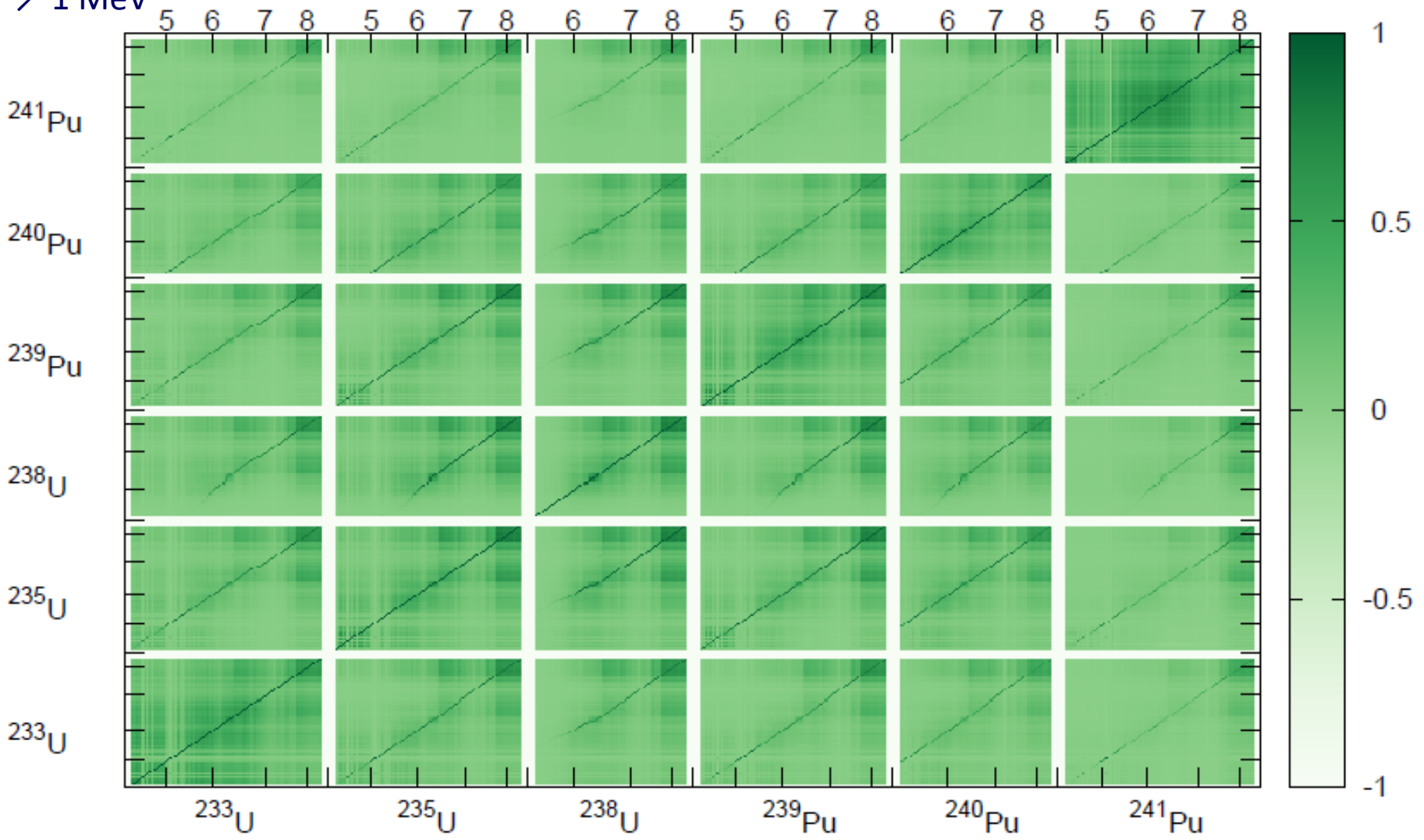
Dashed line: prior

Red line: posterior

Pink area: Uncertainty (50% for prior)

Correlation in Newly Evaluated Cross Sections

"6" → 1 MeV



Compilation of New Cross Sections in ENDF-6 Format

```
JENDL-4.0+SOK                                                          1 0  0     1
 9.223500+4 2.330250+2          1          1          6          19228 1451     1
 0.000000+0 0.000000+0          0          0          0          69228 1451     2
 1.000000+0 2.000000+7          0          0         10          49228 1451     3
 0.000000+0 0.000000+0          0          0        831        1629228 1451     4
 92-U -235 JAEA+                 O.Iwamoto,N.Otuka,S.Chiba,+      9228 1451     5
                                                                  9228 1451     6

----SOK20210404       MATERIAL 9228
-----INCIDENT NEUTRON DATA
------ENDF-6 FORMAT                                                9228 1451     9
                                                                  9228 1451    10

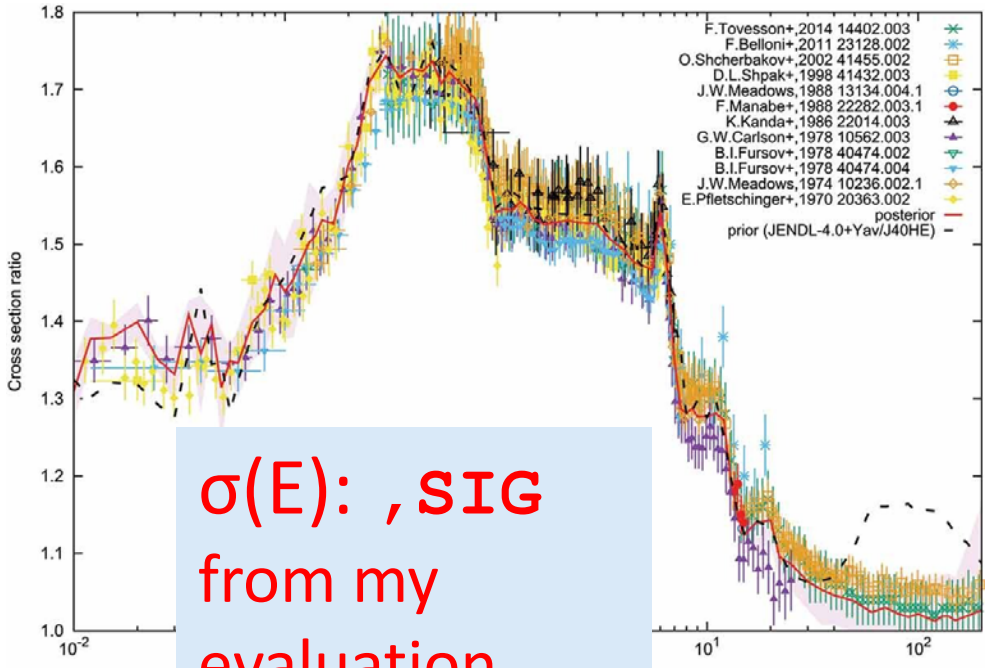
…
 9.223500+4 2.330250+2          0          0          0          09228 3 18     1
 0.000000+0 0.000000+0          0          0          2        3399228 3 18     2
          4          2        339          5                     9228 3 18     3
 1.000000-5 0.000000+0 2.530000-2 0.000000+0 5.000000+2 0.000000+09228 3 18     4
 5.000000+2 1.725620+1 5.029950+2 1.857420+1 5.060080+2 1.958800+19228 3 18     5
…
```

MF3 MT18 = (n,f) cross section

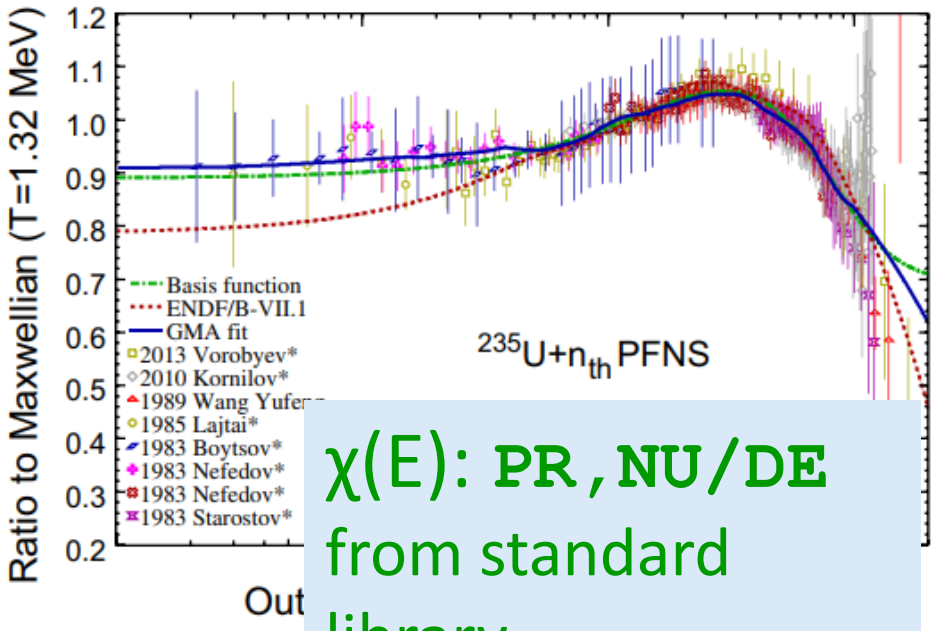
This means σ=17.25620 b at 500 eV, 18.57420 b at 502.9950 eV etc.

This is processed by NJOY for benchmarking (e.g., ^{252}Cf(sf) PFNS SACS, ICSBEP k_{eff})

Validation with PFNS Av. Data (,SIG,,FIS)



σ(E): **,SIG** from my evaluation

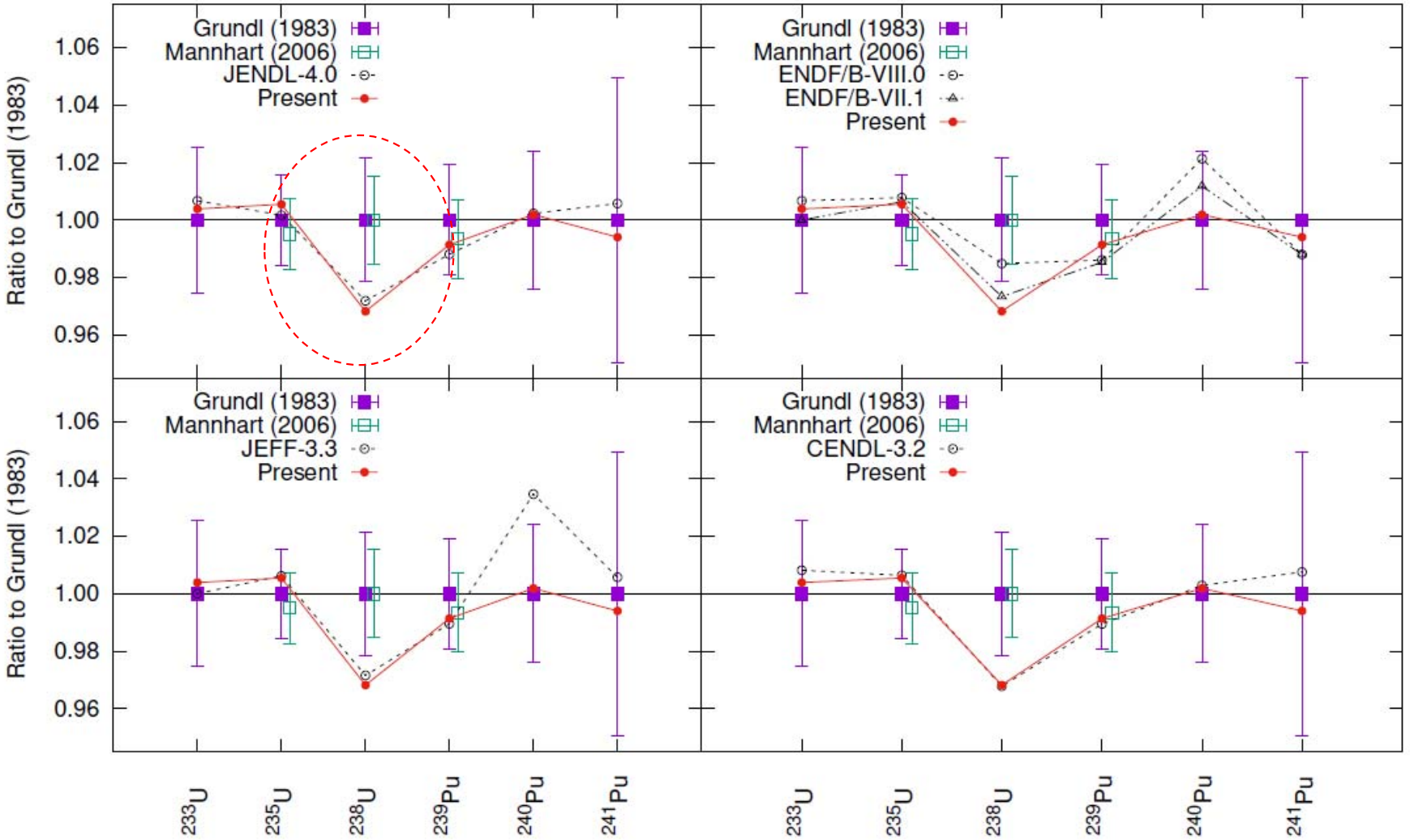


χ(E): **PR,NU/DE** from standard library

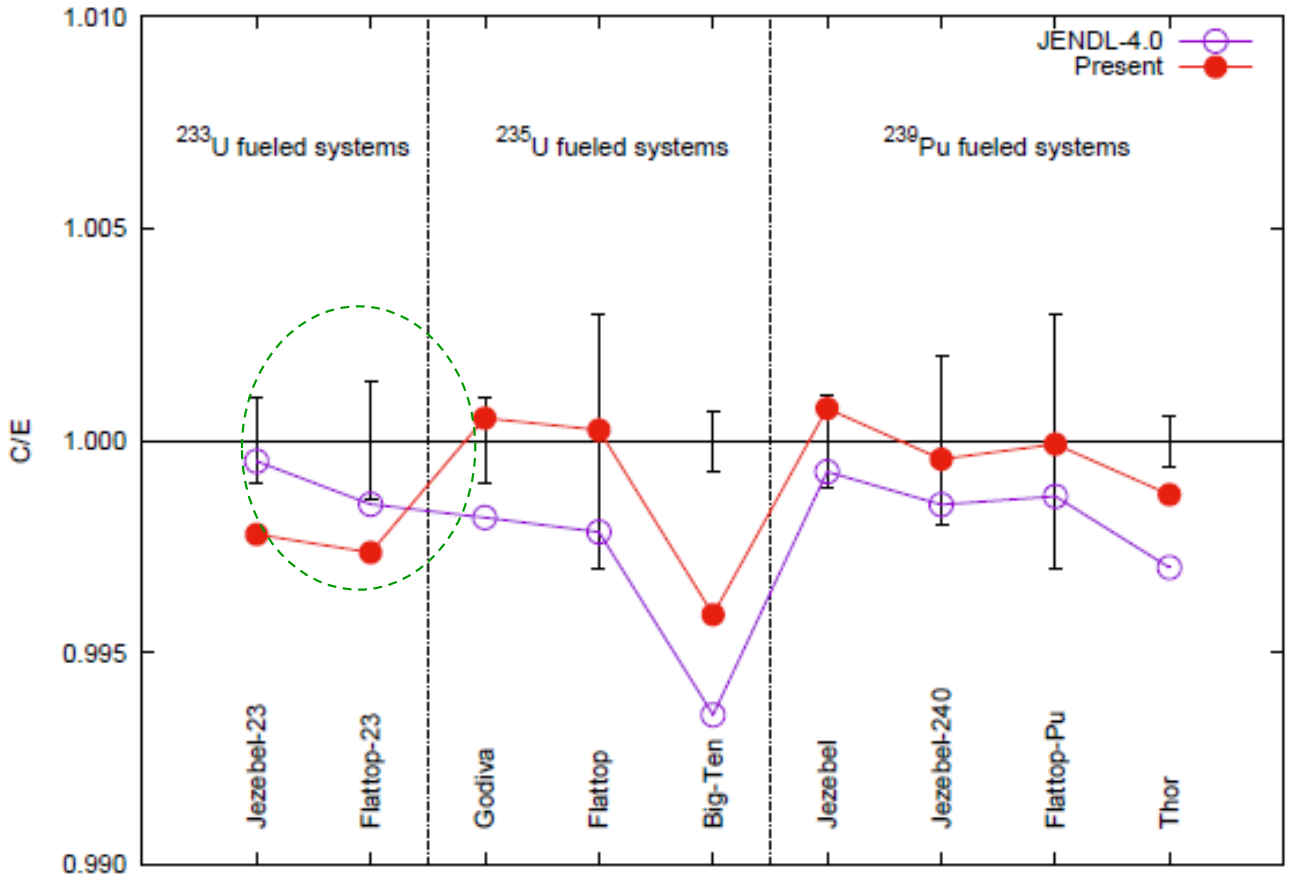
$$\langle\sigma\rangle=\int\sigma(E)\chi(E)\,dE$$

We can compare this with experimental value in EXFOR (compiled as ,SIG,,FIS).

^{252}Cf(sf) SACS (Ratio to Grundl's Exp. SACS)



k_{eff} of LANL Small-Sized Fast Critical Assemblies



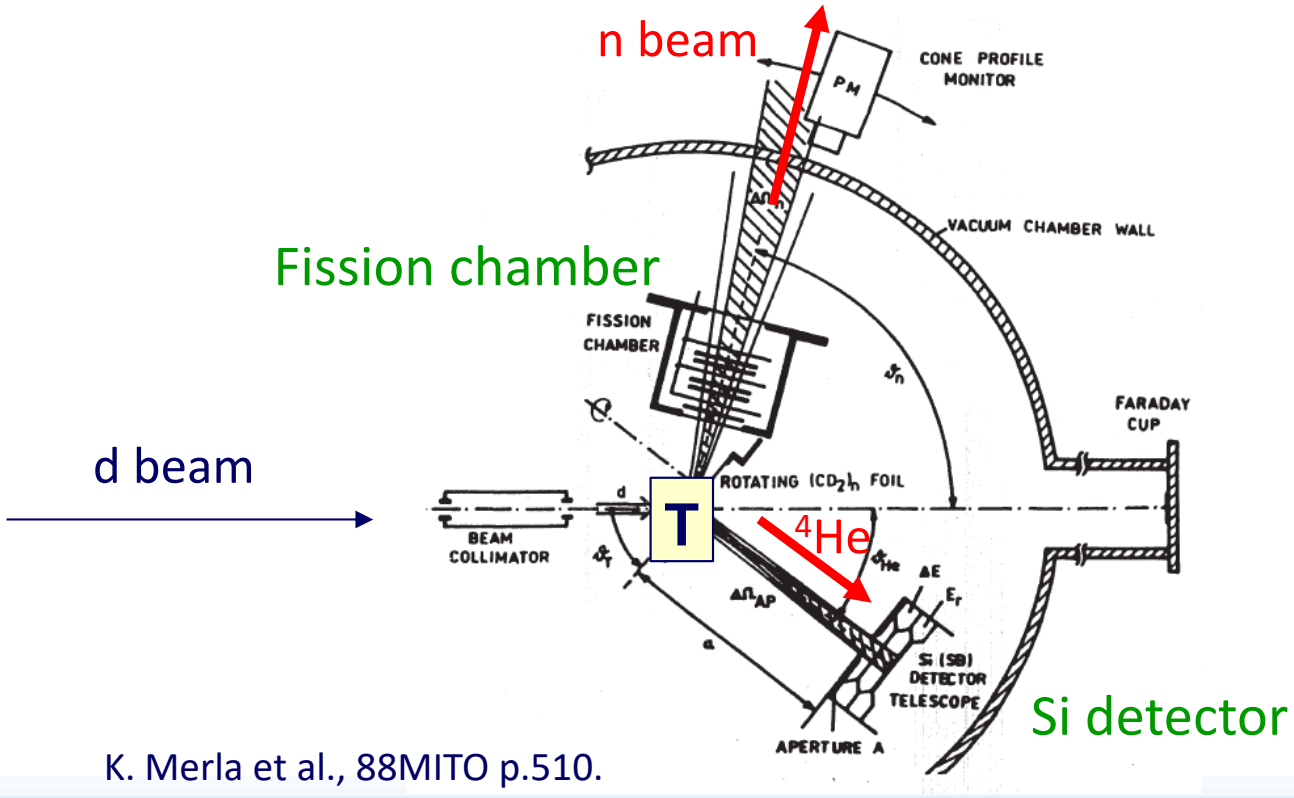
Monte Carlo calculation (MVP) done by Y. Nagaya (JAEA)

The performance of JENDL-5 (adopting new evaluation) for the U-233 systems is better since some quantities other than σ_f were also revised.

Absolute Fission Cross Sections from TUD-KRI Collaboration

Selection of Data from TUD-KRI Collaboration

- TUD (Dresden) and KRI (Leningrad) collaborated for absolute measurements of fission cross sections in 1975-1990.
- Neutron flux was measured by detection of recoil α from $^{3}H(d,n)^{4}He$ (i.e., monitor cross section is not needed.)



K. Merla et al., 88MITO p.510.

Selection of Data from TUD-KRI Collaboration (Cont)

They reported data many times (e.g., ~20 documents for ^{235}U(n,f) at 14 MeV from TUD), and also compiled in EXFOR several times.

Their covariance matrix shows presence of several irradiations. Difficult to choose the final values to be kept in EXFOR.

Repetition of measurements at 14.7 MeV at KRI (RIL) and TUD

Table 1
Covariance matrix of the fission cross-section measurements on ^{235}U

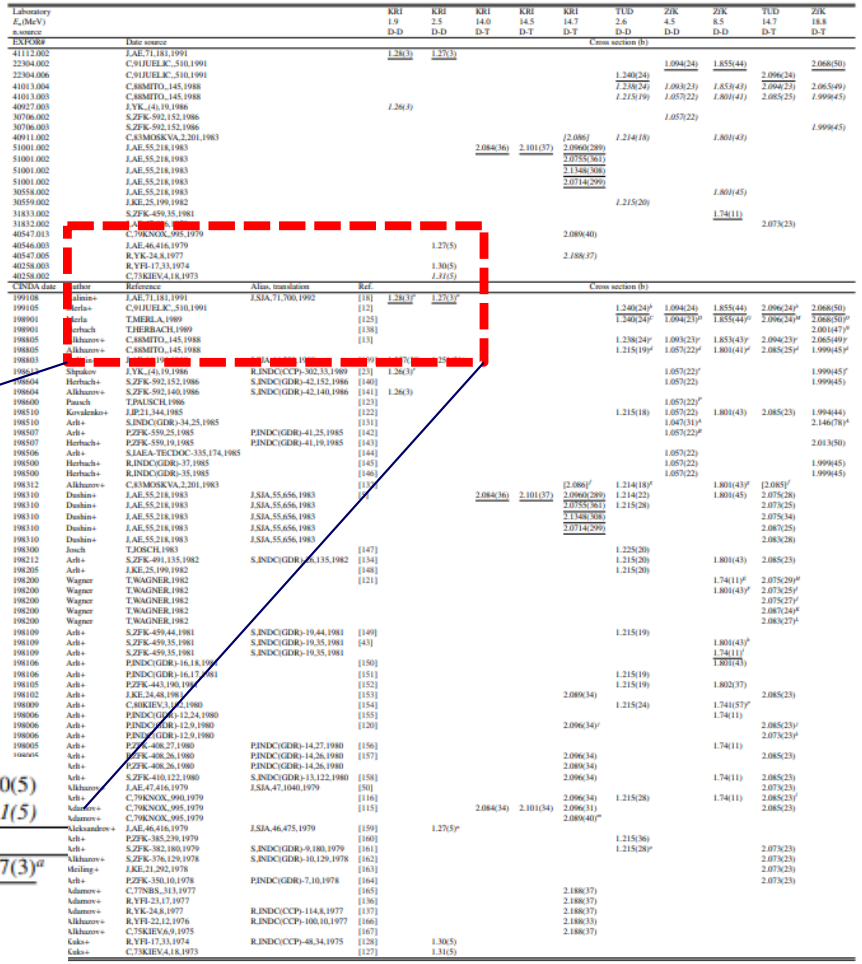
	σ_f (barns)		Covariance matrix (in %^{2})										
RIL	2.0714	(14.7 MeV)	2.08	0.92	0.73	0.82	0.82	0.82	0.41	0.41	0.41	0.41	0.41
RIL	2.1348	(14.7 MeV)		2.08	0.73	0.82	0.82	0.82	0.41	0.41	0.41	0.41	0.41
RIL	2.0755	(14.7 MeV)			3.03	0.67	0.67	0.67	0.45	0.39	0.39	0.39	0.39
RIL	2.0960	(14.7 MeV)				1.90	0.74	0.74	0.31	0.31	0.31	0.31	0.31
RIL	2.1010	(14.5 MeV)					3.02	0.74	0.31	0.31	0.31	0.31	0.31
RIL	2.0840	(14.0 MeV)						3.02	0.31	0.31	0.31	0.31	0.31
TUD	2.083	(14.7 MeV)							1.76	1.05	1.06	1.05	1.06
TUD	2.087	(14.7 MeV)								1.45	1.06	1.05	1.06
TUD	2.075	(14.7 MeV)									2.76	1.05	1.07
TUD	2.073	(14.7 MeV)										1.51	1.06
TUD	2.075	(14.7 MeV)											1.81

V.N.Dushin+, J,SJA,55,656,1983

Selection of Data from TUD-KRI Collaboration (Cont)

We collected all relevant publications compiled in CINDA (manual part) and more (e.g., thesis), and tabulated all values to trace the history of their measurement (for $^{233, 235, 238}$U, ^{239}Pu).

Table 18 of INDC(SEC)-0112 (^{235}U)



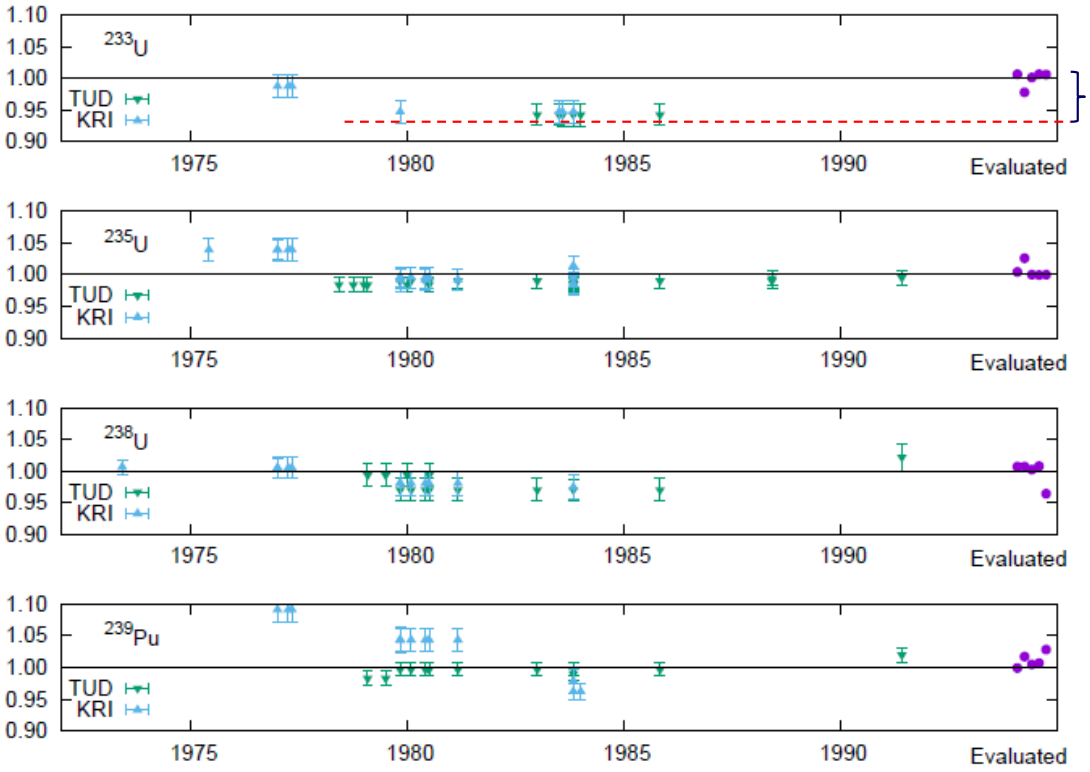
40258.003		R,YFI-17,33,1974				1.30(5)
40258.002		C,73KIEV,4,18,1973				*1.31(5)*
CINDA date	Author	Reference	Alias, translation	Ref.		
199108	Kalinin+	J,AE,71,181,1991	J,SJA,71,700,1992	[18]	1.28(3)[a]	1.27(3)[a]
199105	Merla+	C,91JUELIC,,510,1991		[12]		
198901	Merla	T,MERLA,1989		[125]		
198901	Herbach	T,HERBACH,1989		[138]		
198805	Alkhazov+	C,88MITO,,145,1988		[13]		
198805	Alkhazov+	C,88MITO,,145,1988				
198803	Kalinin+	J,AE,64,194,1988	J,SJA,64,239,1988	[139]	1.257(30)	1.251(31)
198612	Shpakov	J,YK,,(4),19,1986	R,INDC(CCP)-302,33,1989	[23]	1.26(3)[e]	

Selection of Data from TUD-KRI Collaboration (Cont)

Plot of all data in the documents (in or not in EXFOR/CINDA)

X-axis:
Year of publication

Y-axis:
Cross section (relative to my evaluation)



Correction discontinued for ^{233}U

- TUD/ZfK data: Revisions continued till ~1990 by PhD students (Merla, Pausch, Herbach) including experimental study of correction factors with samples returned from KRI.
- KRI data: Revisions finished (stopped?) at ~1984.

Selection of Data from TUD-KRI Collaboration (Cont)

Possible action to CJD and NDS:

Review Tables 17 to 20 of INDC(SEC)-0112, and make necessary revisions in EXFOR entries (addition of SPSDD, move of TUD data from area 4 to 3 and vice versa etc.)

Laboratory		KRI	KRI	KRI	KRI	KRI	TUD	ZfK	ZfK	TUD	ZfK
E_n(MeV)		1.9	2.5	14.0	14.5	14.7	2.6	4.5	8.5	14.7	18.8
n.source		D-D	D-D	D-T	D-T	D-T	D-D	D-D	D-D	D-T	D-T
EXFOR#	Date source	Cross section (b)									
41112.002	J,AE,71,181,1991	1.28(3)	1.27(3)								
22304.002	C,91JUELIC,,510,1991							1.094(24)	1.855(44)		2.068(50)
22304.006	C,91JUELIC,,510,1991						1.240(24)			2.096(24)	
41013.004	C,88MITO,,145,1988						*1.238(24)*	*1.093(23)*	*1.853(43)*	*2.094(23)*	*2.065(49)*
41013.003	C,88MITO,,145,1988						*1.215(19)*	*1.057(22)*	*1.801(41)*	*2.085(25)*	*1.999(45)*
40927.003	J,YK,,(4),19,1986	*1.26(3)*									
30706.002	S,ZFK-592,152,1986							*1.057(22)*			
30706.003	S,ZFK-592,152,1986										*1.999(45)*
40911.002	C,83MOSKVA,2,201,1983					*[2.086]*	*1.214(18)*		*1.801(43)*		
51001.002	J,AE,55,218,1983			2.084(36)	2.101(37)	2.0960(289)					
51001.002	J,AE,55,218,1983					2.0755(361)					
51001.002	J,AE,55,218,1983					2.1348(308)					
51001.002	J,AE,55,218,1983					2.0714(299)					
30558.002	J,AE,55,218,1983								*1.801(45)*		
30559.002	J,KE,25,199,1982						*1.215(20)*				
31833.002	S,ZFK-459,35,1981								1.74(11)		
31832.002	J,AE,47,416,1979									2.073(23)	
40547.013	C,79KNOX,,995,1979					2.089(40)					
40546.003	J,AE,46,416,1979		1.27(5)								
40547.005	R,YK-24,8,1977					*2.188(37)*					
40258.003	R,YFI-17,33,1974		1.30(5)								
40258.002	C,73KIEV,4,18,1973		*1.31(5)*								
CINDA date	Author Reference Alias translation Ref						Cross section (b)				

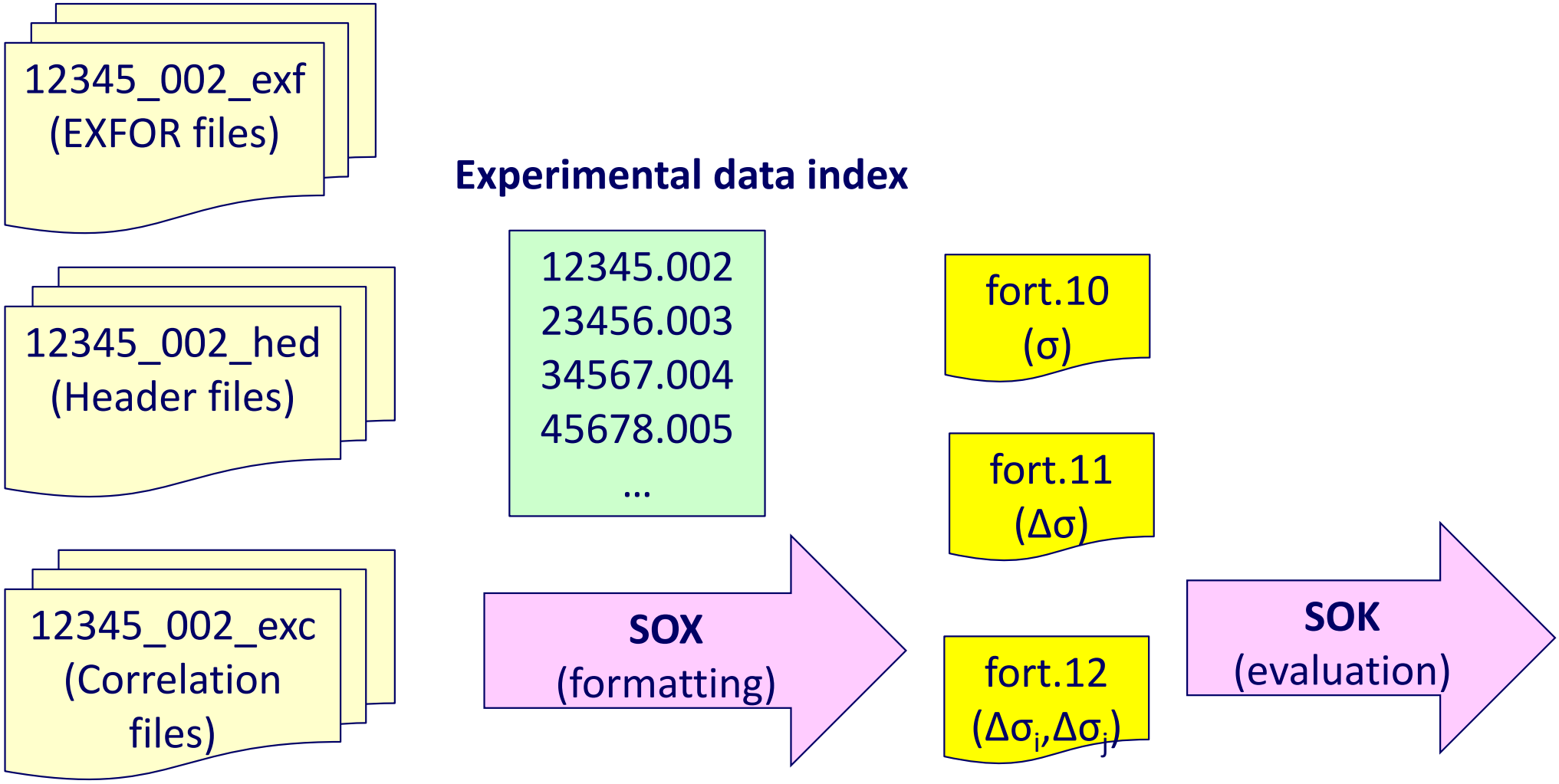
Direct Use of EXFOR Files in Least-Squares Analysis

Comparison of This Evaluation and IAEA STD Evaluation

	Present (~JENDL-5)	IAEA-STD 2017
Tool	SOK	GMA (+ R-matrix tools)
Reaction	^{233,235,238}U, ^{239,240,241}Pu(n,f)	^{235,238}U, ^{239}Pu(n,f), ^{6}Li(n,t)^{4}He, ^{10}B(n,α)^{7}Li and more
Linearization	Log transformation	First order Taylor approximation
Grid structure	Not necessary to be common	Common in all reactions
Experimental database	EXFOR (original with minimum corrections)	GMA database (original data may be modified by experienced evaluators)

Flow of Data from EXFOR Entries to SOK Input

(X4Pro may replace EXFOR Files.)



Experimental Input Files

Data index file (list of experimental datasets – subentry# + pointer)

```
%235U(n,f):7.0E+03:2.5E+08:1.0:3.5:RT:1.0:2.4:RB
P92235.018                                  JENDL-4.0
 51006.002   20201215  1.0000E+00 2ZZZCER  S.Amaducci+,2019    # instead of 23453.002.2+003.2
#23453.002.2 20201203  1.0000E+00 2ZZZCER  S.Amaducci+,2019    # Not for JENDL4. Use 51006.002.
#23453.003.2 20201203  1.0000E+00 2ZZZCER  S.Amaducci+,2019    # Not for JENDL4. Use 51006.002.
 23078.002   20201217  1.0000E+00 2BLGLVN+ R.Nolte+,2007       # Not for JENDL4, HE
```

EXFOR (EXF) file
(original EXFOR)

```
SUBENT     C    23078002    20201217
BIB                   8           25
REACTION    (92-U-235(N,F),,SIG)
…
ENDBIB               25            0
NOCOMMON              0            0
DATA                  6            9
EN          EN-ERR      DATA        ERR-T       MISC        FLAG
MEV         MEV         B           B           MEV         NO-DIM
 32.80       0.16        2.08        0.12        32.74       1.
 33.00       0.18        2.10        0.11        32.74       1.
 44.91       0.24        1.97        0.14        45.27       1.
…
```

Header (HED) file
(correlation property etc.)

```
 EN
 EN
 EN-ERR
 DATA

 ERR-T       U
 ERR-1       1.
 ERR-2       1.
 ERR-4       1.
…
```

This means that the residual uncertainty is **U**ncorrelated

Experimental Input Files (cont)

Correlation file (correlation coefficients)

```
#14498.002   R.J.Casperson+,2018                72
 1.000
 0.713 1.000
 0.713 0.730 1.000
 0.717 0.735 0.737 1.000
 0.717 0.731 0.730 0.739 1.000
 0.708 0.728 0.736 0.738 0.735 1.000
 0.710 0.726 0.729 0.738 0.731 0.735 1.000
 0.705 0.726 0.733 0.735 0.726 0.731 0.737 1.000
 0.695 0.712 0.725 0.728 0.716 0.718 0.719 0.718 1.000
 0.677 0.692 0.697 0.702 0.693 0.701 0.700 0.699 0.693 1.000
 0.640 0.660 0.667 0.679 0.663 0.671 0.675 0.672 0.658 0.646 1.000
 0.642 0.669 0.662 0.671 0.662 0.672 0.673 0.669 0.660 0.638 0.625 1.000
 0.646 0.654 0.666 0.669 0.671 0.671 0.676 0.676 0.663 0.648 0.611 0.617
 1.000
…
```

A correlation file is crated only when the correlation coefficients tabulated by the experimentalists are available (Typically coded under COVARIANCE in EXFOR entries.)

SOX output (=Experimental Input of SOK)

fort.10 (experimental cross section: E_1, σ_1, E_2, σ_2, …)

```
23078.002   R.Nolte+,2007                          8
3.2800E+07 2.0800E+00 3.3000E+07 2.1000E+00 4.4910E+07 1.9700E+00
5.9950E+07 1.7200E+00 5.9950E+07 1.9600E+00 9.6500E+07 1.9300E+00
1.4700E+08 1.4000E+00 1.9900E+08 1.3800E+00
```

fort.11 (experimental total uncertainty E_1, $\Delta\sigma_1$, E_2, $\Delta\sigma_2$, …)

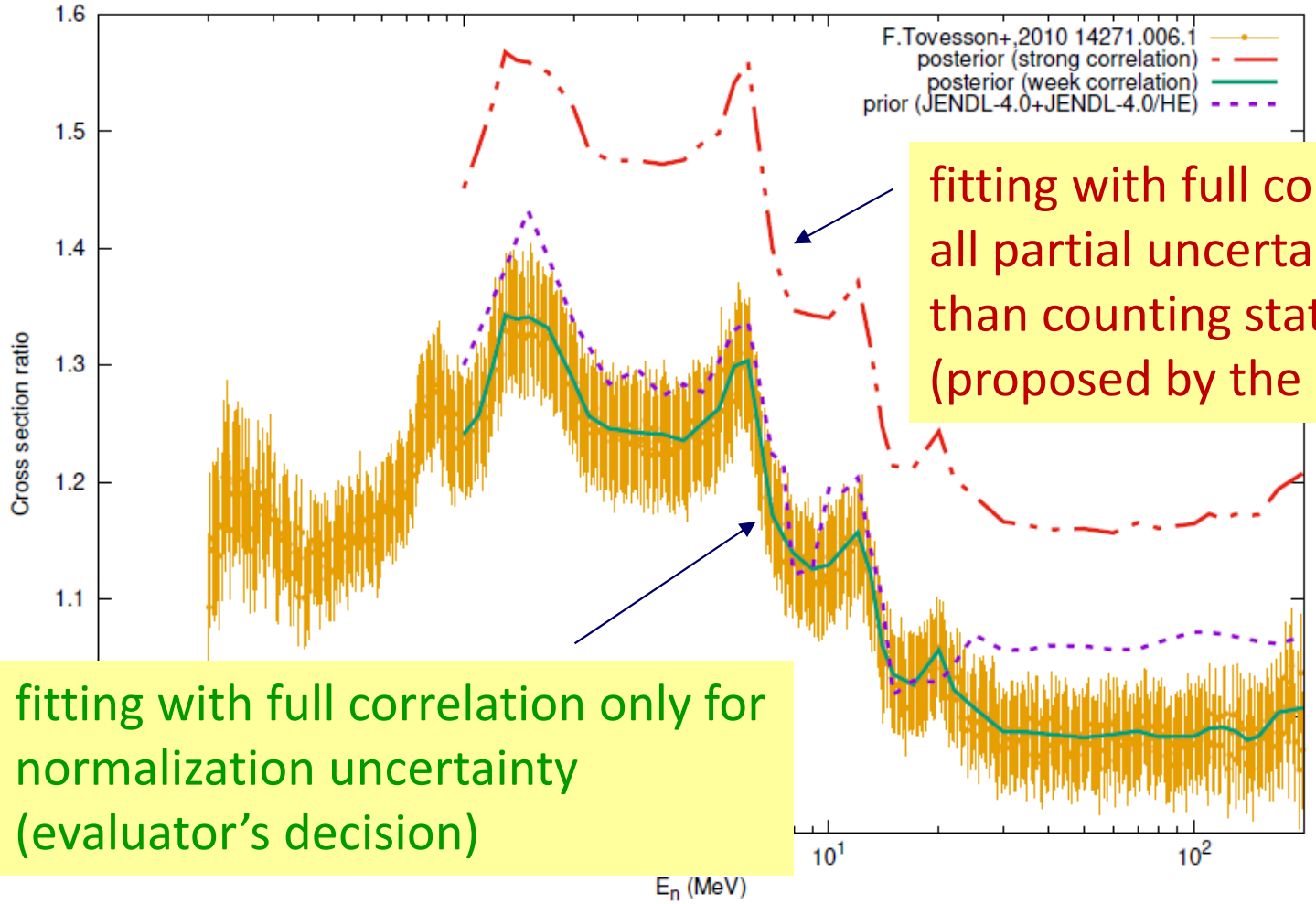
```
23078.002   R.Nolte+,2007                          8
3.2800E+07 5.7692E-02 3.3000E+07 5.2381E-02 4.4910E+07 7.1066E-02
5.9950E+07 5.8140E-02 5.9950E+07 6.1224E-02 9.6500E+07 1.0881E-01
1.4700E+08 9.2857E-02 1.9900E+08 8.6957E-02
```

fort.12 (experimental correlation coefficients)

```
23078.002   R.Nolte+,2007                          8
1.000
0.567 1.000
0.418 0.460 1.000
0.511 0.562 0.415 1.000
0.485 0.534 0.394 0.481 1.000
0.273 0.301 0.222 0.271 0.257 1.000
0.320 0.352 0.260 0.317 0.301 0.170 1.000
0.341 0.376 0.277 0.339 0.322 0.181 0.212 1.000
```

Impact of Correlation Properties Assigned by Evaluator

$^{241}Pu(n,f)/^{235}U(n,f)$ measured by F. Tovesson et al. at LANCE (EXFOR 14271.006.1)



fitting with full correlation for all partial uncertainties other than counting statistics (proposed by the authors)

fitting with full correlation only for normalization uncertainty (evaluator's decision)

EXFOR-to-SOK Input Conversion Log

```
*  23078.002   20201217  1.0000E+00 2BLGLVN+ R.Nolte+,2007
1 flagged data lines skipped.
23078.002  :ERR-T     :  :   : 5.2%:10.9%:Total uncertainty e
section (5%) but including the uncertainties due to
23078.002  :ERR-1     :MU:1.0: 0.2%: 0.2%:Number of fissionab
23078.002  :ERR-2     :  :1.0: 1.6%: 1.6%:Chamber efficiency (1.6%)
23078.002  :ERR-4     :MU:1.0: 2.5%: 2.5%:Peak fluence (2.5-3.5%)
23078.002  :ERR-5     :  :1.0: 2.0%: 2.0%:Monitor readings (2%)
23078.002  :ERR-6     :  :1.0: 0.7%: 0.7%:Neutron transport in fiss.chamber(0.7%)
23078.002  :ERR-7     :  :1.0: 0.9%: 0.9%:Fragment loss below threshold (0.9%)
23078.002  :ERR-8     :  :1.0: 0.4%: 0.4%:Dead time (0.4%)
23078.002  :ERR-9     :  :1.0: 0.2%: 0.2%:Telescope - fiss.chamber distance(0.2%)
23078.002  :ERR-10    :  :1.0: 0.3%: 0.3%:Neutron absorption in air (0.3%)
23078.002  :ERR-11    :  :1.0: 1.3%: 1.3%:Inhomogeneity of neutron fluence (1.3%)
23078.002  :ERR-12    :MU:1.0: 1.0%: 1.0%:Fiss. due to low-energy neutrons (1-7%)
23078.002  :ERR-R     :RU:0.0: 3.2%:10.1%:Residual uncertainty (specified as un
```

Free text under ERR-ANALYS
(Compiler's input is important!)

```
(ERR-1,0.2,0.5) Number of fissionable nuclei (0.2-0.5%)
(ERR-2)         Chamber efficiency              (1.6%)
(ERR-3,1.,5.)   Number of fission events        (1-5%)
(ERR-4,2.5,3.5) Peak fluence                  (2.5-3.5%)
…
```

Correlation coefficients assigned by the evaluator

Making correlation property assigned by the evaluator traceable!

EXFOR-to-SOK Input Conversion Log (cont)

```
*  23078.002   20201217  1.0000E+00 2BLGLVN+ R.Nolte+,2007

1 flagged data lines skipped.

23078.002  :ERR-T      :  :    : 5.2
cross section (5%) but including t

23078.002  :ERR-1      :MU:1.0: 0.2

23078.002  :ERR-2      :  :1.0: 1.6

23078.002  :ERR-4      :MU:1.0: 2.5

23078.002  :ERR-5      :  :1.0: 2.0

23078.002  :ERR-6      :  :1.0: 0.7

23078.002  :ERR-7      :  :1.0: 0.9

23078.002  :ERR-8      :  :1.0: 0.4

23078.002  :ERR-9      :  :1.0: 0.2

23078.002  :ERR-10     :  :1.0: 0.3

23078.002  :ERR-11     :  :1.0: 1.3

23078.002  :ERR-12     :MU:1.0: 1.0

23078.002  :ERR-R      :RU:0.0: 3.2
```

^{233}U cross sections

EXFOR 23072.009 (M.Calviani+,2009)					
ERR-C	CT		2.9%	3.3%	Total uncertainty (calculated)
ERR-S		0.0	0.8%	1.8%	Statistical uncertainty
ERR-1		1.0	1.8%	1.8%	Sample mass (1.8%)
ERR-2		1.0	1.5%	1.5%	Pulse height threshold (1.5%)
ERR-3		1.0	1.0%	1.0%	Dead-time correction (1.0%)
ERR-4		1.0	1.0%	1.0%	Normalization to ^{235}U(n,f) (1.0%-2.0%)
EXFOR 22698.005 (F.Tovesson+,2004)					
ERR-T			1.8%	2.1%	Combined systematic and statistical error
ERR-1		1.0	1.4%	1.4%	^{237}Np mass (1.4%)
ERR-2		1.0	1.0%	1.0%	^{237}Np(n,f) cross section (1%)
ERR-R	RU	0.0	0.4%	1.2%	Residual uncertainty (specified as uncorrelated)
EXFOR 13890.004 (K.H.Guber+,2000)					
ERR-C	CT		1.0%	1.1%	Total uncertainty (calculated)
ERR-S		0.0	0.2%	0.5%	Statistical uncertainty
ERR-A	AU	1.0	1.0%	1.0%	Normalization uncertainty from 22080.002 (0.25% from thermal normalization+0.7% from point-wise uncertainty)
EXFOR 40927.002 (V.I.Shpakov,1986)					
ERR-T			3.6%	3.6%	Total error
ERR-S		0.0	2.9%	2.9%	Statistical error
ERR-R	RU	1.0	2.1%	2.1%	Residual uncertainty (specified as fully corre-

The log file was converted to LaTeX and published to make our evaluation more traceable in the future (c.f. Table 16 of INDC(SEC)-0112 (Rev.))

Distribution of SOK Input Files from Publisher

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*************************************************************************
*
* Experimental datasets
* for simultaneous evaluation of 233,235,238U and 239,240,241Pu(n,f)
* cross sections for JENDL-5
*
* This is a supplemental material of
*
*  Naohiko Otuka, Osamu Iwamoto
*  "EXFOR-based simultaneous evaluation of neutron-induced uranium and
*   plutonium fission cross sections for JENDL-5"
*  Journal of Nuclear Science and Technology Vol.59 (2022)
*  http://doi.org/10.1080/00223131.2022.2030259
*
* A sample Fortran source code is followed by cross section data lines
```

One can freely download the experimental data input files converted from EXFOR as "supplemental materials" of publisher's website.

Summary

- Simultaneous evaluation of ^{233,235,238}U, ^{239,240,241}Pu(n,f) till 200 MeV with SOK
- Direct use of EXFOR source files
- Many EXFOR entries were revised in collaboration with other neutron data centres to make covariance related information (e.g., partial uncertainties) machine readable!
- In-depth analysis of fission cross sections from TUD-KRI collaboration (EXFOR entries still need to be revied and updated for some cases.)
- An effort was made to make this evaluation traceable
- Work in progress for fission cross sections of other actinides in fast region.

Acknowledgement